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USPAT2 NEWS 9 JAN 13 IPC 8 searching in IFIPAT, IFIUDB, and IFICDB

New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to NEWS 10 JAN 13 INPADOC

Pre-1988 INPI data added to MARPAT NEWS 11 JAN 17

IPC 8 in the WPI family of databases including WPIFV NEWS 12 JAN 17

NEWS 13 JAN 30 Saved answer limit increased

NEWS 14 JAN 31 Monthly current-awareness alert (SDI) frequency added to TULSA

JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01, NEWS EXPRESS CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT http://download.cas.org/express/v8.0-Discover/

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=> file registry COST IN U.S. DOLLARS

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FULL ESTIMATED COST

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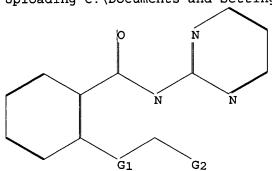
\*\*\*\*\*\*\*\*\*\*\* The CA roles and document type information have been removed from \* \* the IDE default display format and the ED field has been added, \* effective March 20, 2005. A new display format, IDERL, is now available and contains the CA role and document type information. \*\*\*\*\*\*\*\*\*\*\*\*\*\*

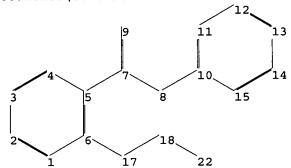
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=> Uploading C:\Documents and Settings\jballs\My Documents\10-629817G.str





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212

chain nodes : 7 8 9 17 18 19 20 21 ring nodes : 12 13 14 15 1 2 3 4 5 6 10 11

chain bonds : 7-9 8-10 17-18 18-22 19-20 5-7 6-17 7-8

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3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds :

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exact bonds :

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normalized bonds :

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G2:0, [\*1], [\*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:CLASS

#### L1 STRUCTURE UPLOADED

=> s l1 sub sam

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SEARCH ENDED BY USER

=> s l1

SAMPLE SEARCH INITIATED 14:10:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 106 TO 614
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> file caplus

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ENTRY SESSION
FULL ESTIMATED COST
0.88
1.09

FILE 'CAPLUS' ENTERED AT 14:11:14 ON 14 FEB 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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=> s l1 sam

REG1stRY INITIATED

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SAMPLE SEARCH INITIATED 14:11:39 FILE 'REGISTRY'
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100.0% PROCESSED 18 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 106 TO 614

PROJECTED ANSWERS: 0 TO 0

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L4 0 L3

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Substance data SEARCH and crossover from CAS REGISTRY in progress...
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100.0% PROCESSED 18 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 106 TO 614

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L1

L6 0 L5

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REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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100.0% PROCESSED 340 ITERATIONS 7 ANSWERS

SEARCH TIME: 00.00.01

L7 7 SEA SSS FUL L1

L8 5 L7

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         2000:457059 CAPLUS
DN
         133:89437
         Preparation of heteroaryl-substituted aromatic amides as factor Xa
 TΙ
         inhibitors
         Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman;
 IN
         Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven
         Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine
         Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez,
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         Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton;
         Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
         Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
 PA
         PCT Int. Appl., 403 pp.
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LA
         English
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                                                      DATE
                                                                        APPLICATION NO.
                                                                                                                 DATE
         PATENT NO.
                                    7.1
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US 6759414 B2 20040706

US 2005282862 A1 20051222

PRAI US 1998-113556P P 19981223

WO 1999-US29946 W

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                        ALL CITATIONS AVAILABLE IN THE RE FORMAT
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         ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
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 ACCESSION NUMBER:
                                           133:89437
 DOCUMENT NUMBER:
                                           Entered STN: 07 Jul 2000
 ENTRY DATE:
                                           Preparation of heteroaryl-substituted aromatic amides
 TITLE:
                                           as factor Xa inhibitors
                                           Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl
 INVENTOR(S):
                                           Penman; Franciskovich, Jeffry Bernard; Goodson,
                                           Theodore, Jr.; Hall, Steven Edward; Herron, David
                                           Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine
                                           Joseph; Masters, John Joseph; Mendel, David; Milot,
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Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
PATENT ASSIGNEE(S):
SOURCE:
                           PCT Int. Appl., 403 pp.
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DOCUMENT TYPE:
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LANGUAGE:
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INT. PATENT CLASSIF.:
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                           C07D401-14
       SECONDARY:
                           C07D401-12; C07D417-14; C07D409-14; C07D405-14;
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                           A61P007-02; C07D401-14; C07D213-00; C07D213-00;
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MARPAT 133:89437
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OTHER SOURCE(S): GRAPHIC IMAGE:

#### ABSTRACT:

The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

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SUPPL. TERM: arom amide heteroaryl prepn formulation factor Xa inhibitor
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anticoagulant

INDEX TERM: Anticoagulants

(preparation of heteroaryl-substituted aromatic amides as factor

Xa inhibitors)

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ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

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                               280773-94-6P
                                               280773-96-8P
               280773-93-5P
280773-97-9P
               280773-98-0P
                               280773-99-1P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
```

INDEX TERM:

```
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)
```

INDEX TERM:

280774-00-7P 280774-01-8P 280774-02-9P 280774-03-0P 280774-04-1P 280774-05-2P 280774-06-3P 280774-07-4P

280774-08-5P 280774-09-6P 280774-15-4P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted aromatic amides as factor

Xa inhibitors)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS

RECORD.

REFERENCE(S): (1) Beight Douglas Wade; WO 9900121 A 1999 CAPLUS

- (2) Beight Douglas Wade; WO 9900128 A 1999 CAPLUS
- (3) Berlex Lab; WO 9628427 A 1996 CAPLUS
- (4) Katakura; EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY
  CHIMICA THERAPEUTICA 1995, V30(5), P387 CAPLUS
- (5) Kunitada, S; CURRENT PHARMACEUTICAL DESIGN 1996, V2(5),

P6

(6) Schering Ag; WO 9932477 A 1999 CAPLUS

#### => d ibib abs 1

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:457059 CAPLUS

DOCUMENT NUMBER: 133:89437

TITLE: Preparation of heteroaryl-substituted aromatic amides

as factor Xa inhibitors

INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl

Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert;

Yee, Ying Kwong

PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.

SOURCE: PCT Int. Appl., 403 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.			KIND DATE				APPLICATION NO.			DATE							
WO	2000	0391	18		A1		2000	0706		WO 1	L999-1	US29:	946		1	9991:	215
	₩:	ΑE,	AL,	AM,	AT,	AU,	ΑZ,	BA,	ΒB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
		CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,
		IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚŻ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,
		MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,
		SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	ŪG,	US,	UΖ,	VN,	YU,	ZA,	zw	
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,
		DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,
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CA	2361	149			AA		2000	0706		CA 1	L999-	2361	149		1	9991:	215
EP	1140	903			Al		2001	1010		EP 1	1999-	9642	79		1	9991:	215
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					LV,												
JP	2002	5334	54		T2		2002	1008		JP 2	2000-	5910	29		1	9991:	215
	2726						2004	0815		AT 3	L999-	9642	79		1	9991:	215
ES	2226						2005	0316		-	L999-						
US	6635	657			В1		2003	1021		US 2	2001-	8577	51		2	0010	608
US	2004	0298	74		Al		2004	0212	•	US 2	2003 -	6297	60		- 2	0030	729
US	6759	414			В2		2004	0706									
US	2005	2828	62		A1		2005	1222			2003-						
PRIORIT	Y APP	LN.	INFO	.:						US 1	1998-	1135	56P		P 1	9981	223

OTHER SOURCE(S):

MARPAT 133:89437

GI

The title compds. [I; A3-A6, together with the two carbons to which they AΒ are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 =H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un) substituted at the 5-position, 3-pyridinyl (un) substituted at the 6-position, 2-pyrimidinyl (un) substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; <math>Q2 =(un) substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day. REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

L3

L4

L5

L6

(FILE 'HOME' ENTERED AT 14:09:38 ON 14 FEB 2006)

FILE 'REGISTRY' ENTERED AT 14:09:53 ON 14 FEB 2006

STRUCTURE UPLOADED L1L20 S L1

> FILE 'CAPLUS' ENTERED AT 14:11:14 ON 14 FEB 2006 S L1

FILE 'REGISTRY' ENTERED AT 14:11:39 ON 14 FEB 2006 0 S L1 SAM

FILE 'CAPLUS' ENTERED AT 14:11:39 ON 14 FEB 2006

0 S L3 SAM S L1

FILE 'REGISTRY' ENTERED AT 14:12:03 ON 14 FEB 2006

FILE 'CAPLUS' ENTERED AT 14:12:03 ON 14 FEB 2006

0 S L5 S L1

FILE 'REGISTRY' ENTERED AT 14:12:25 ON 14 FEB 2006 7 S L1 FULL L7

FILE 'CAPLUS' ENTERED AT 14:12:26 ON 14 FEB 2006 L8 5 S L7 FULL

=> d l8 ibib abs

ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2000:457059 CAPLUS

DOCUMENT NUMBER:

133:89437

TITLE: Preparation of heteroaryl-substituted aromatic amides

as factor Xa inhibitors

INVENTOR(S):

Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong

PATENT ASSIGNEE(S):

Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al. PCT Int. Appl., 403 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

English

1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA			KIND DATE		APPLICATION NO.				DATE								
WO	2000									WO	1999-	US29:					215
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		CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD	), GE,	GH,	GM,	HR,	HU	ID,	IL,
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		SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG	US,	UZ,	VN,	YU,	ZA,	ZW	
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	ΤZ	, UG,	ZW,	AT,	BE,	CH	CY,	DE,
		DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU	, MC,	NL,	PT,	SE,	BF	ВJ,	CF,
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CA	2361	149			AA		2000	0706		CA	1999-	2361	149		-	19991	215
EP	1140	903			A1		2001	1010		ΕP	1999-	9642	79		:	19991	215
EP	1140	903			B1		2004	0804									
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO										
JP	2002	5334	54		T2		2002	1008		JΡ	2000-	5910:	29		:	19991	215
								0815		ΑT	1999-	9642	79			19991	215
ES	2226	485			Т3		2005	0316		ES	1999-	9642	79			19991	215
US	6635	657			B1		2003	1021		US	2001-	8577	51		2	20010	608
US	2004	0298	74		A1		2004	0212		US	2003-	6297	60		2	20030	729
US	6759	414			B2		2004	0706									
US	2005	2828	62		Al		2005	1222		US	2003-	6298	17		2	20030	729
PRIORITY	Y APP	LN.	INFO	. :						US	1998-	1135	56P	]	Ρ :	19981	223
										WO	1999-	US29:	946	V	N :	19991	215
										US	2001-	8577	51	7	A3 2	20010	608

OTHER SOURCE(S):

MARPAT 133:89437

AB The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

II

```
6
REFERENCE COUNT:
=> 1
1 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).
=> d his
     (FILE 'HOME' ENTERED AT 14:09:38 ON 14 FEB 2006)
     FILE 'REGISTRY' ENTERED AT 14:09:53 ON 14 FEB 2006
                STRUCTURE UPLOADED
L_1
L2
              0 S L1
     FILE 'CAPLUS' ENTERED AT 14:11:14 ON 14 FEB 2006
                S L1
     FILE 'REGISTRY' ENTERED AT 14:11:39 ON 14 FEB 2006
              0 S L1 SAM
L3
     FILE 'CAPLUS' ENTERED AT 14:11:39 ON 14 FEB 2006
              0 S L3 SAM
L4
                S L1
     FILE 'REGISTRY' ENTERED AT 14:12:03 ON 14 FEB 2006
              0 S L1
L5
     FILE 'CAPLUS' ENTERED AT 14:12:03 ON 14 FEB 2006
              0 S L5
L6
                S L1
     FILE 'REGISTRY' ENTERED AT 14:12:25 ON 14 FEB 2006
              7 S L1 FULL
L7
     FILE 'CAPLUS' ENTERED AT 14:12:26 ON 14 FEB 2006
              5 S L7 FULL
L8
=> d 17 ibib abs 1-7
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y
'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
The following are valid formats:
Substance information can be displayed by requesting individual
fields or predefined formats. The predefined substance formats
are: (RN = CAS Registry Number)
```

SAM - Index Name, MF, and structure - no RN FIDE - All substance data, except sequence data IDE - FIDE, but only 50 names SQIDE - IDE, plus sequence data SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used - Protein sequence data, includes RN SOD SQD3 - Same as SQD, but 3-letter amino acid codes are used - Protein sequence name information, includes RN SON CALC - Table of calculated properties

- Table of experimental properties EPROP - EPROP and CALC PROP

REG

- RN

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats

# must be cited first. The CA File predefined formats are: ABS -- Abstract APPS -- Application and Priority Information BIB -- CA Accession Number, plus Bibliographic Data CAN -- CA Accession Number CBIB -- CA Accession Number, plus Bibliographic Data (compressed) IND -- Index Data IPC -- International Patent Classification PATS -- PI, SO STD -- BIB, IPC, and NCL IABS -- ABS, indented, with text labels IBIB -- BIB, indented, with text labels ISTD -- STD format, indented OBIB ----- AN, plus Bibliographic Data (original) OIBIB ----- OBIB, indented with text labels SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available. The MAX format is the same as ALL. The IALL format is the same as ALL with BIB ABS and IND indented, with text labels. For additional information, please consult the following help messages: HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats. ENTER DISPLAY FORMAT (IDE):ide ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN L7 856975-07-0 REGISTRY RN Entered STN: 26 Jul 2005 ED Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) CN INDEX NAME) 3D CONCORD FS C20 H18 N4 O4 MF CAS EARLY REGISTRATIONS SR STN Files: CA, CAPLUS Ph-CH2-Me

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L7 ANSWER 2 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
  RN 349622-99-7 REGISTRY
  ED Entered STN: 01 Aug 2001
  CN Benzamide 2-(acetylamino)-N-(4.6-dimethyl-2-pyrimidinyl)- (90
- CN Benzamide, 2-(acetylamino)-N-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

  FS 3D CONCORD
- MF C15 H16 N4 O2
- SR Chemical Library

Supplier: MicroChemistry Ltd.

LC STN Files: CHEMCATS

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 280768-70-9 REGISTRY

ED Entered STN: 27 Jul 2000

CN 4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phe

nyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H21 Cl N6 O2

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 267891-53-2 REGISTRY

ED Entered STN: 02 Jun 2000

CN Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI)

(CA INDEX NAME)

FS 3D CONCORD

MF C21 H16 Cl N5 O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L7 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 267891-24-7 REGISTRY
- ED Entered STN: 02 Jun 2000
- CN Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI)
  - (CA INDEX NAME)
- FS 3D CONCORD
- MF C17 H14 Cl N5 O
- SR CA
- LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L7 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 180206-29-5 REGISTRY
- ED Entered STN: 29 Aug 1996
- CN Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX
- NAME)
- FS 3D CONCORD
- MF C32 H27 N3 O4
- SR CA
- LC STN Files: CA, CAPLUS

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L7 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 69589-68-0 REGISTRY
- ED Entered STN: 16 Nov 1984
- CN Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)
- FS 3D CONCORD
- MF C18 H14 N4 O2
- LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT
  - (\*File contains numerically searchable property data)

```
N NH-C-Ph
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### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d his

L1

L2

L3

L4

L5

L6

L7

L8

(FILE 'HOME' ENTERED AT 14:09:38 ON 14 FEB 2006)

FILE 'REGISTRY' ENTERED AT 14:09:53 ON 14 FEB 2006

STRUCTURE UPLOADED

0 S L1

FILE 'CAPLUS' ENTERED AT 14:11:14 ON 14 FEB 2006 S L1

FILE 'REGISTRY' ENTERED AT 14:11:39 ON 14 FEB 2006 0 S L1 SAM

FILE 'CAPLUS' ENTERED AT 14:11:39 ON 14 FEB 2006

0 S L3 SAM

S L1

FILE 'REGISTRY' ENTERED AT 14:12:03 ON 14 FEB 2006

0 S L1

FILE 'CAPLUS' ENTERED AT 14:12:03 ON 14 FEB 2006

0 S L5

S L1

FILE 'REGISTRY' ENTERED AT 14:12:25 ON 14 FEB 2006

7 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:12:26 ON 14 FEB 2006

5 S L7 FULL

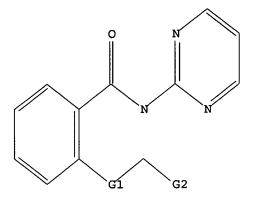
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FILE 'CAPLUS' ENTERED AT 14:14:57 ON 14 FEB 2006

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O, N G2 O, [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

#### => logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:Y COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

0.00

FULL ESTIMATED COST

0.46 196.02

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

-2.25

CA SUBSCRIBER PRICE

ENTRY SESSION

STN INTERNATIONAL LOGOFF AT 14:15:26 ON 14 FEB 2006

Connection closed by remote host

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSPTARJB1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America

NEWS 2 "Ask CAS" for self-help around the clock

NEWS 3 DEC 05 CASREACT(R) - Over 10 million reactions available

NEWS 4 DEC 14 2006 MeSH terms loaded in MEDLINE/LMEDLINE

NEWS 5 DEC 14 2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER

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NEWS 6 DEC 14 CA/Caplus to be enhanced with updated IPC codes
                IPC search and display fields enhanced in CA/CAplus with the
NEWS 7 DEC 21
                IPC reform
        DEC 23 New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
NEWS
     8
                USPAT2
                IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS 9
        JAN 13
NEWS 10 JAN 13 New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to
                INPADOC
NEWS 11 JAN 17 Pre-1988 INPI data added to MARPAT
NEWS 12 JAN 17 IPC 8 in the WPI family of databases including WPIFV
NEWS 13 JAN 30 Saved answer limit increased
NEWS 14 JAN 31 Monthly current-awareness alert (SDI) frequency
                added to TULSA
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NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT
http://download.cas.org/express/v8.0-Discover/

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 14:36:32 ON 14 FEB 2006

=> file registry
COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
0.42 0.42

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:37:27 ON 14 FEB 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 FEB 2006 HIGHEST RN 874180-50-4 DICTIONARY FILE UPDATES: 13 FEB 2006 HIGHEST RN 874180-50-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

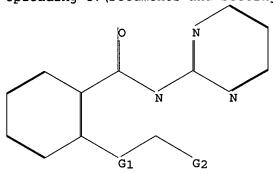
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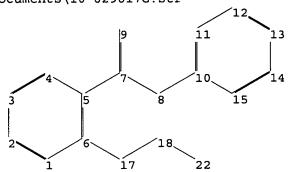
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>\_

Uploading C:\Documents and Settings\jballs\My Documents\10-629817G.str





cy<sup>2</sup>

119

212

chain nodes :

7 8 9 17 18 19 20 21 22

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15

chain bonds :

5-7 6-17 7-8 7-9 8-10 17-18 18-22 19-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds :

6-17 7-8 7-9 8-10 17-18 18-22 19-20

exact bonds :

5-7

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

G1:0,N

G2:O,[\*1],[\*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:CLASS

### L1 STRUCTURE UPLOADED

=> s 11

SAMPLE SEARCH INITIATED 14:38:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED SEARCH TIME: 00.00.01 18 ITERATIONS

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

106 TO PROJECTED ITERATIONS: 0

O TO PROJECTED ANSWERS:

0 SEA SSS SAM L1 1.2

=> file CAPLUS

SINCE FILE TOTAL COST IN U.S. DOLLARS

> ENTRY SESSION 0.86

FULL ESTIMATED COST 0.44

FILE 'CAPLUS' ENTERED AT 14:38:12 ON 14 FEB 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 14 Feb 2006 VOL 144 ISS 8 FILE LAST UPDATED: 13 Feb 2006 (20060213/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l1

### REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:38:17 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -18 TO ITERATE

18 ITERATIONS 0 ANSWERS 100.0% PROCESSED

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

\*\*COMPLETE\*\* BATCH 106 TO 614

PROJECTED ITERATIONS: PROJECTED ANSWERS: 0 TO 0

0 SEA SSS SAM L1

0 L3

=> s 11 full

# REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures. FULL SEARCH INITIATED 14:38:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 340 TO ITERATE

100.0% PROCESSED 340 ITERATIONS

SEARCH TIME: 00.00.06

L5 7 SEA SSS FUL L1

L6 5 L5

=> d 15 all abs

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L5 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 856975-07-0 REGISTRY

ED Entered STN: 26 Jul 2005

CN Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA

7 ANSWERS

INDEX NAME)

FS 3D CONCORD

SR

MF C20 H18 N4 O4

CAS EARLY REGISTRATIONS

LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

## Ring System Data

			Ring System		RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
=======	, +=======-	+========-		+========	+=======
C6	C6	6		46.150.18	
C4N2	NCNC3	6	C4N2	46.195.39	1

$$\begin{array}{c|c} \text{Me} & \text{O} & \text{NO}_2 \\ \hline & \text{N} & \text{NH-C} \\ \hline & \text{Ph-CH}_2-\text{O} \\ \\ & \text{Me} \end{array}$$

## Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
=======================================	+=========	+========	+====
Bioconc. Factor (BCF)	4.89	pH 1	(1)
Bioconc. Factor (BCF)	238	pH 4	(1)
Bioconc. Factor (BCF)	248	pH 7	(1)
Bioconc. Factor (BCF)	230	pH 8	(1)
Bioconc. Factor (BCF)	25.6	pH 10	(1)
Freely Rotatable Bonds (FRB)	7		(1)
H acceptors (HAC)	8		(1)
H donors (HD)	1	1	(1)

```
35.4
                                                pH 1
                                                              (1)
Koc (KOC)
                                                pH 4
                                                              (1)
                               1726
Koc (KOC)
                                                pH 7
                               1797
                                                              (1)
Koc (KOC)
                                                pH 8
Koc (KOC)
                               1666
                                                              (1)
                                                pH 10
                                                              (1)
Koc (KOC)
                               185
                                                pH 1
logD (LOGD)
                               1.75
                                                              (1)
                                                |pH 4
                               3.44
                                                              (1)
logD (LOGD)
                                                pH 7
                               3.45
                                                              (1)
logD (LOGD)
                                                8 Hq
logD (LOGD)
                               3.42
                                                              (1)
                                                pH 10
logD (LOGD)
                               2.47
                                                              (1)
                               3.460+/-0.596
logP (LOGP)
                                                              (1)
Molar Solubility (SLB.MOL)
                               0.00037 mol/L
                                                |pH 1
                                                              (1)
Molar Solubility (SLB.MOL)
                               |0.0000076 mol/L|pH 4
                                                              (1)
Molar Solubility (SLB.MOL)
                               0.0000073 mol/L|pH 7
                                                              (1)
Molar Solubility (SLB.MOL)
                               0.0000078 mol/L|pH 8
                                                              (1)
                               0.000070 mol/L |pH 10
Molar Solubility (SLB.MOL)
                                                              (1)
Molecular Weight (MW)
                               378.38
                                                              (1)
                               9.05 + / - 0.70
                                                Most Acidic (1)
pKa (PKA)
                               2.70+/-0.17
                                                |Most Basic | (1)
pKa (PKA)
```

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V4.76 ((C) 1994-2006 ACD/Labs)

Tuberculostatic derivatives of p-aminobenzoic acid. III. Heterocyclic

See HELP PROPERTIES for information about property data sources in REGISTRY.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

47:22216 CA

AN

ΤI

```
derivatives of 4-aminosalicylic acid
     Jensen, Kai Arne; Ingvorsen, Helmuth
ΑU
     Univ. Copenhagen
CS
     Acta Chemica Scandinavica (1952), 6, 161-5
SO
     CODEN: ACHSE7; ISSN: 0904-213X
DT
     Journal
     English
LA
     10 (Organic Chemistry)
CC
     cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and
AΒ
     4-aminosalicylic acid (II) were prepared, including 4-nitro-
     salicylomorpholide (III), m. 247-8°, and -piperidide (IV), m.
     230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and
     -piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m.
     170° and 4-aminobenzoic acid (VIII), m. 160°;
     2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X),
     m. 178°, and -benzanilide (XI), m. 201°;
     4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'-
     nitrobenzamido)pyridine (XIII), m. 144°, -thiazole (XIV), m.
     201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and
     -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4-
     aminobenzamido)pyridine (XVII), m. 183°, -thiazole (XVIII), m.
     214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et
     4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at
     120°, the excess XX removed at 100° in vacuo, the residue
     dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving
     50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g.
     PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional
     crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly
     prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were
     refluxed until colorless, 0.2 N NaOH added until the color reappeared, the
     EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII
     (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction
     of the NO2 gave VIII. VII (10 g.) and 10 cc. SOCl2 were refluxed 1-1.5
     h., the excess SOC12 was removed in vacuo, and the IX (9.2 g.) treated
     with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in
     30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9
     g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into
     300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the
```

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solution filtered, part of the EtOH removed in vacuo, H2O added, the solution
heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI
were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9
g. acid chloride. XVII to XIX were obtained by hydrogenation of the
corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro
compds. at 100° and 150 atmospheric gave the corresponding azoxy compds.
Heterocyclic compounds
Heterocyclic compounds
Heterocyclic compounds
Heterocyclic compounds
Salicylamide, 4-nitro-N-2-pyridyl-
Salicylamide, N-(5-methyl-1,3,4-thiadiazol-2-yl)-4-nitro-
Salicylanilide, 4-nitro-4'-sulfamoyl-
65-49-6, Salicylic acid, 4-amino-
                                   150-13-0, Benzoic acid, p-amino-
   (derivs.)
                                                 6935-15-5, Salicylic
5340-21-6, Benzoic acid, 2-(benzyloxy)-4-nitro-
acid, 4-carboxyamino-, 4-benzyl ester 39614-82-9, Salicyloyl chloride, 4-nitro- 78154-65-1, Salicylanilide, 4-amino- 78154-68-4, Morpholine
                                                  78154-68-4, Morpholine,
4-(4-nitrosalicyloyl)-
                         78154-68-4, Phenol, 2-morpholinocarbonyl-5-nitro-
   78154-69-5, Piperidine, 1-(4-nitrosalicyloyl)-
                                                    78154-69-5, Phenol,
5-nitro-2-piperidinocarbonyl- 78154-70-8, Morpholine,
                         78154-71-9, Phenol, 5-amino-2-piperidinocarbonyl-
4-(4-aminosalicyloyl)-
   78154-71-9, Piperidine, 1-(4-aminosalicyloyl)-
                                                    99072-94-3,
Salicylamide, 4-amino-N-(5-methyl-1,3,4-thiadiazol-2-yl)-
                                                             99185-78-1,
Salicylamide, 4-amino-N-2-thiazolyl-
                                      99989-22-7, Salicylamide,
4-amino-N-2-pyridyl-
                      100872-84-2, Benzamide, 2-(benzyloxy)-4-nitro-
106952-12-9, Salicylanilide, 4',4'''-sulfonylbis[4-amino- 109016-83-3,
Salicylanilide, 4-amino-4'-sulfamoyl-
                                        193803-83-7, Benzoic acid,
4-amino-2-(benzyloxy)-
                        607713-82-6, Benzoyl chloride,
2-(benzyloxy)-4-nitro-
                         721920-30-5, 5-Thiazolecarboxylic acid,
4-methyl-2-(4-nitrosalicylamido)-, ethyl ester 850852-03-8, Thiazole,
2-[2-(benzyloxy)-4-nitrobenzamido]- 856848-98-1, Pyridine,
2-[2-(benzyloxy)-4-nitrobenzamido]- 856861-93-3, Salicylamide,
                            856975-07-0, Pyrimidine, 2-[2-(benzyloxy)-4-
4-nitro-N-s-triazol-3-yl-
                                857533-50-7, Benzanilide,
nitrobenzamido] -4,6-dimethyl-
4-amino-2-(benzyloxy)-
                        857534-05-5, Benzanilide, 2-(benzyloxy)-4-nitro-
857748-51-7, 1,3,4-Thiadiazole, 2-[4-amino-2-(benzyloxy)benzamido]-5-
          857748-52-8, 1,3,4-Thiadiazole, 2-[2-(benzyloxy)-4-
                            857749-06-5, 1,3,4-Thiadiazole,
nitrobenzamido]-5-methyl-
2-methyl-5-[N4-(4-nitrosalicyloyl)sulfanilamido]-
                                                    857749-06-5,
Salicylanilide, 4'-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfamoyl]-4-nitro-
857756-40-2, Salicylamide, N-(4,5-dimethyl-2-thiazolyl)-4-nitro-
48-0, Salicylamide, 4-nitro-N-p-sulfamoylbenzyl- 857756-83-3,
Salicylanilide, 4-amino-4'-(2-thiazolylsulfamoyl)-
                                                      857757-02-9,
Salicylanilide, 4'-[(4-methyl-2-pyrimidinyl)sulfamoyl]-4-nitro-
                                                                   857757-0
2-9, Pyrimidine, 4-methyl-2-[N4-(4-nitrosalicyloyl)sulfanilamido]-
                                                                   857757-0
857757-06-3, Salicylanilide, 4-nitro-4'-(2-thiazolylsulfamoyl)-
6-3, Thiazole, 2-[N4-(4-nitrosalicyloyl)sulfanilamido]-
                                                           858479-10-4,
Salicylamide, 4-nitro-N-2-thiazolyl- 858479-45-5, Salicylamide,
4-amino-N-p-sulfamoylbenzyl-
                               858479-46-6, Salicylanilide,
4-nitro-4'-(2-pyrimidinylsulfamoyl)-
                                      858479-47-7, Salicylanilide,
4-nitro-4'-(2-pyridylsulfamoyl)- 858479-65-9, Salicylanilide,
4-amino-4'-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfamoyl]-
                                                          858479-65-9,
1,3,4-Thiadiazole, 2-[N4-(4-aminosalicyloyl)sulfanilamido]-5-methyl-
                                                              860507-31-9,
859466-83-4, Thiazole, 2-[4-amino-2-(benzyloxy)benzamido]-
                                                       860507-36-4,
Salicylamide, 4-amino-N-(4,5-dimethyl-2-thiazolyl)-
Salicylanilide, 4',4'''-sulfonylbis[4-nitro-
                                               867131-41-7, Pyridine,
                                     873401-46-8, 1,3,4-Thiadiazole,
2-[4-amino-2-(benzyloxy)benzamido]-
2-methyl-5-(4-nitrosalicylamido)-
   (preparation of)
cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and
4-aminosalicylic acid (II) were prepared, including 4-nitro-
salicylomorpholide (III), m. 247-8°, and -piperidide (IV), m.
230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and
-piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m.
170° and 4-aminobenzoic acid (VIII), m. 160°;
2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X),
m. 178°, and -benzanilide (XI), m. 201°;
4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'-
nitrobenzamido)pyridine (XIII), m. 144°, -thiazole (XIV), m.
```

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AB

201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4aminobenzamido)pyridine (XVII), m. 183°, -thiazole (XVIII), m. 214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et 4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at 120°, the excess XX removed at 100° in vacuo, the residue dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving 50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g. PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were refluxed until colorless, 0.2 N NaOH added until the color reappeared, the EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction of the NO2 gave VIII. VII (10 g.) and 10 cc. SOCl2 were refluxed 1-1.5 h., the excess SOC12 was removed in vacuo, and the IX (9.2 g.) treated with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in 30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9 g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into 300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the solution filtered, part of the EtOH removed in vacuo, H2O added, the solution heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9 q. acid chloride. XVII to XIX were obtained by hydrogenation of the corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro compds. at 100° and 150 atmospheric gave the corresponding azoxy compds.

### => s l1 full 2

#### REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:39:39 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\* PROJECTED ITERATIONS: 106 TO 614 PROJECTED ANSWERS: O TO 0

0 SEA SSS SAM L1 L7

0 L7 L8

MISSING OPERATOR L8 FULL The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> d l1 full 2 L1 HAS NO ANSWERS 'FULL ' IS NOT A VALID STRUCTURE FORMAT KEYWORD Structure Formats SIA ---- Structure Image, Attributes, and map table if it contains data. (Default) SIM ---- Structure IMage. SAT ---- Structure ATtributes and map table if it contains data. SCT ---- Structure Connection Table and map table if it contains

data.

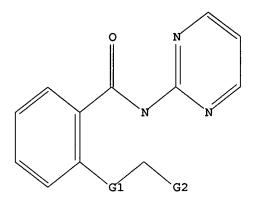
SDA ---- All Structure DAta (image, attributes, connection table and

map table if it contains data).

NOS ----- NO Structure data.

ENTER STRUCTURE FORMAT (SIM), NOS:sim

L1 STR



Cy Cy

G1 O, N G2 O, [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

=> d 15 ibib abs 1-7
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY' 'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN

SAM - Index Name, MF, and structure - no RN FIDE - All substance data, except sequence data

IDE - FIDE, but only 50 names SQIDE - IDE, plus sequence data

SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used

SQD - Protein sequence data, includes RN

SQD3 - Same as SQD, but 3-letter amino acid codes are used

SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties EPROP - Table of experimental properties

PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

APPS -- Application and Priority Information

BIB -- CA Accession Number, plus Bibliographic Data

```
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL
IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels
SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.
For additional information, please consult the following help
messages:
HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):ide
     ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
L5
     856975-07-0 REGISTRY
RN
     Entered STN: 26 Jul 2005
ED
     Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI)
CN
     INDEX NAME)
FS
     3D CONCORD
     C20 H18 N4 O4
MF
     CAS EARLY REGISTRATIONS
SR
                  CA, CAPLUS
     STN Files:
LC
            NH-
             Ph-CH_2-O
      Me
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
               1 REFERENCES IN FILE CA (1907 TO DATE)
               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
     ANSWER 2 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
L5
     349622-99-7 REGISTRY
RN
     Entered STN: 01 Aug 2001
ED
     Benzamide, 2-(acetylamino)-N-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA
CN
     INDEX NAME)
     3D CONCORD
FS
     C15 H16 N4 O2
ΜF
SR
     Chemical Library
       Supplier: MicroChemistry Ltd.
     STN Files:
                  CHEMCATS
LC
```

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 280768-70-9 REGISTRY

ED Entered STN: 27 Jul 2000

CN 4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phe

nyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H21 Cl N6 O2

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 267891-53-2 REGISTRY

ED Entered STN: 02 Jun 2000

CN Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI)

(CA INDEX NAME)

FS 3D CONCORD

MF C21 H16 C1 N5 O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 267891-24-7 REGISTRY

ED Entered STN: 02 Jun 2000

CN Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI)

(CA INDEX NAME)

FS 3D CONCORD

C17 H14 Cl N5 O

SR CA

MF

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 180206-29-5 REGISTRY

ED Entered STN: 29 Aug 1996

CN Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX

NAME)

FS 3D CONCORD

MF C32 H27 N3 O4

SR CA

LC STN Files: CA, CAPLUS

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 69589-68-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H14 N4 O2

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

(\*File contains numerically searchable property data)

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### => d 15 all 1-7

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y) /N:y

L5 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 856975-07-0 REGISTRY

ED Entered STN: 26 Jul 2005

CN Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA

INDEX NAME)

FS 3D CONCORD

MF C20 H18 N4 O4

SR CAS EARLY REGISTRATIONS

LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

# Ring System Data

		Size of the Rings SZ	Ring System Formula RF	Ring  Identifier   RID	RID Occurrence Count
C6	+======-   C6   NCNC3	6		46.150.18   46.195.39	

$$\begin{array}{c|c} \text{Me} & \text{N} & \text{NO}_2 \\ \hline & \text{N} & \text{NH-C} \\ \hline & \text{Ph-CH}_2-\text{O} \\ \\ \text{Me} & \end{array}$$

# Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	\=====================================	рн 1	(1)
	238	<b>4</b>	(1)
	248	pH 7	(1)
Bioconc. Factor (BCF)	230	8 Hq	(1)

Bioconc. Factor (BCF)	25.6	рн 10	(1)
Freely Rotatable Bonds (FRB)	7		(1)
H acceptors (HAC)	8		(1)
H donors (HD)	1		(1)
Koc (KOC)	35.4	pH 1	(1)
Koc (KOC)	1726	pH 4	(1)
Koc (KOC)	1797	рн 7	(1)
Koc (KOC)	1666	рн 8	(1)
Koc (KOC)	185	рн 10	(1)
logD (LOGD)	1.75	рн 1	(1)
logD (LOGD)	3.44	pH 4	(1)
logD (LOGD)	3.45	pH 7	(1)
logD (LOGD)	3.42	8 Hq	(1)
logD (LOGD)	2.47	pH 10	(1)
logP (LOGP)	3.460+/-0.596		(1)
Molar Solubility (SLB.MOL)	0.00037 mol/L	pH 1	(1)
Molar Solubility (SLB.MOL)	0.0000076 mol/L	!	(1)
Molar Solubility (SLB.MOL)	0.0000073 mol/L	: -	(1)
	0.0000078 mol/L	! -	(1)
Molar Solubility (SLB.MOL)	!	рн 10	(1)
Molecular Weight (MW)	378.38	10	(1)
	1	  Most Acidic	
pKa (PKA)	! "		(1)
pKa (PKA)	[2.70+/-0.17	Inosc paste	1 ( ± /

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V4.76 ((C) 1994-2006 ACD/Labs)

Tuberculostatic derivatives of p-aminobenzoic acid. III. Heterocyclic

See HELP PROPERTIES for information about property data sources in REGISTRY.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

AN

47:22216 CA

derivatives of 4-aminosalicylic acid

```
Jensen, Kai Arne; Ingvorsen, Helmuth
AU
CS
    Univ. Copenhagen
    Acta Chemica Scandinavica (1952), 6, 161-5
SO
     CODEN: ACHSE7; ISSN: 0904-213X
DT
    Journal
    English
LΑ
CC
     10 (Organic Chemistry)
     cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and
AΒ
     4-aminosalicylic acid (II) were prepared, including 4-nitro-
     salicylomorpholide (III), m. 247-8°, and -piperidide (IV), m.
     230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and
     -piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m.
     170° and 4-aminobenzoic acid (VIII), m. 160°;
     2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X),
     m. 178°, and -benzanilide (XI), m. 201°;
     4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'-
     nitrobenzamido)pyridine (XIII), m. 144°, -thiazole (XIV), m.
     201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and
     -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4-
     aminobenzamido)pyridine (XVII), m. 183°, -thiazole (XVIII), m.
     214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et
     4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at
     120°, the excess XX removed at 100° in vacuo, the residue
     dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving
     50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g.
     PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional
     crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly
     prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were
     refluxed until colorless, 0.2 N NaOH added until the color reappeared, the
     EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII
     (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction
     of the NO2 gave VIII. VII (10 g.) and 10 cc. SOC12 were refluxed 1-1.5
     h., the excess SOCl2 was removed in vacuo, and the IX (9.2 g.) treated
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with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in
 30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9
 g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into
 300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the
 solution filtered, part of the EtOH removed in vacuo, H2O added, the solution
 heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI
 were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9
 g. acid chloride. XVII to XIX were obtained by hydrogenation of the
 corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro
 compds. at 100° and 150 atmospheric gave the corresponding azoxy compds.
 Heterocyclic compounds
 Heterocyclic compounds
 Heterocyclic compounds
 Heterocyclic compounds
 Salicylamide, 4-nitro-N-2-pyridyl-
 Salicylamide, N-(5-methyl-1,3,4-thiadiazol-2-yl)-4-nitro-
 Salicylanilide, 4-nitro-4'-sulfamoyl-
                                    150-13-0, Benzoic acid, p-amino-
 65-49-6, Salicylic acid, 4-amino-
    (derivs.)
 5340-21-6, Benzoic acid, 2-(benzyloxy)-4-nitro- 6935-15-5, Salicylic
 acid, 4-carboxyamino-, 4-benzyl ester 39614-82-9, Salicyloyl chloride,
            78154-65-1, Salicylanilide, 4-amino- 78154-68-4, Morpholine,
                          78154-68-4, Phenol, 2-morpholinocarbonyl-5-nitro-
 4-(4-nitrosalicyloyl)-
    78154-69-5, Piperidine, 1-(4-nitrosalicyloyl)-
                                                     78154-69-5, Phenol,
 5-nitro-2-piperidinocarbonyl- 78154-70-8, Morpholine,
                          78154-71-9, Phenol, 5-amino-2-piperidinocarbonyl-
 4-(4-aminosalicyloyl)-
    78154-71-9, Piperidine, 1-(4-aminosalicyloyl)- 99072-94-3,
                                                              99185-78-1,
 Salicylamide, 4-amino-N-(5-methyl-1,3,4-thiadiazol-2-yl)-
 Salicylamide, 4-amino-N-2-thiazolyl- 99989-22-7, Salicylamide,
                       100872-84-2, Benzamide, 2-(benzyloxy)-4-nitro-
 4-amino-N-2-pyridyl-
 106952-12-9, Salicylanilide, 4',4'''-sulfonylbis[4-amino- 109016-83-3,
                                         193803-83-7, Benzoic acid,
 Salicylanilide, 4-amino-4'-sulfamoyl-
 4-amino-2-(benzyloxy)-
                          607713-82-6, Benzoyl chloride,
                         721920-30-5, 5-Thiazolecarboxylic acid,
 2-(benzyloxy)-4-nitro-
 4-methyl-2-(4-nitrosalicylamido)-, ethyl ester 850852-03-8, Thiazole,
 2-[2-(benzyloxy)-4-nitrobenzamido]- 856848-98-1, Pyridine, 2-[2-(benzyloxy)-4-nitrobenzamido]- 856861-93-3, Salicylamide,
                             856975-07-0, Pyrimidine, 2-[2-(benzyloxy)-4-
 4-nitro-N-s-triazol-3-yl-
                                 857533-50-7, Benzanilide,
 nitrobenzamido] -4,6-dimethyl-
                         857534-05-5, Benzanilide, 2-(benzyloxy)-4-nitro-
 4-amino-2-(benzyloxy)-
 857748-51-7, 1,3,4-Thiadiazole, 2-[4-amino-2-(benzyloxy)benzamido]-5-
           857748-52-8, 1,3,4-Thiadiazole, 2-[2-(benzyloxy)-4-
                             857749-06-5, 1,3,4-Thiadiazole,
 nitrobenzamido]-5-methyl-
 2-methyl-5-[N4-(4-nitrosalicyloyl) sulfanilamido] -
                                                     857749-06-5,
 Salicylanilide, 4'-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfamoyl]-4-nitro-
 857756-40-2, Salicylamide, N-(4,5-dimethyl-2-thiazolyl)-4-nitro-
                                                                     857756-
 48-0, Salicylamide, 4-nitro-N-p-sulfamoylbenzyl- 857756-83-3,
 Salicylanilide, 4-amino-4'-(2-thiazolylsulfamoyl)-
                                                      857757-02-9,
 Salicylanilide, 4'-[(4-methyl-2-pyrimidinyl)sulfamoyl]-4-nitro-
                                                                    857757-0
 2-9, Pyrimidine, 4-methyl-2-[N4-(4-nitrosalicyloyl)sulfanilamido]-
 857757-06-3, Salicylanilide, 4-nitro-4'-(2-thiazolylsulfamoyl)-
                                                                    857757-0
 6-3, Thiazole, 2-[N4-(4-nitrosalicyloyl)sulfanilamido]-
                                                            858479-10-4,
 Salicylamide, 4-nitro-N-2-thiazolyl- 858479-45-5, Salicylamide,
                                858479-46-6, Salicylanilide,
 4-amino-N-p-sulfamoylbenzyl-
 4-nitro-4'-(2-pyrimidinylsulfamoyl)-
                                       858479-47-7, Salicylanilide,
 4-nitro-4'-(2-pyridylsulfamoyl)-
                                   858479-65-9, Salicylanilide,
 4-amino-4'-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfamoyl]-
                                                            858479-65-9,
 1,3,4-Thiadiazole, 2-[N4-(4-aminosalicyloyl)sulfanilamido]-5-methyl-
                                                               860507-31-9,
 859466-83-4, Thiazole, 2-[4-amino-2-(benzyloxy)benzamido]-
 Salicylamide, 4-amino-N-(4,5-dimethyl-2-thiazolyl)-
                                                        860507-36-4,
 Salicylanilide, 4',4'''-sulfonylbis[4-nitro-867131-41-7, Pyridine,
 2-[4-amino-2-(benzyloxy)benzamido]- 873401-46-8, 1,3,4-Thiadiazole,
 2-methyl-5-(4-nitrosalicylamido)-
    (preparation of)
ANSWER 2 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
 349622-99-7 REGISTRY
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Benzamide, 2-(acetylamino)-N-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA

IT

IT

ΙT

Ļ5 RN

ED

CN

Entered STN: 01 Aug 2001

INDEX NAME)

FS 3D CONCORD MF C15 H16 N4 O2 SR Chemical Library

Supplier: MicroChemistry Ltd.

LC STN Files: CHEMCATS

# Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
ΕĀ	ES	SZ	RF	RID	Count
	-========	-========+	·======+		
C6	C6	6		46.150.18	
C4N2	NCNC3	6	C4N2	46.195.39	1

# Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE		OTE
Bioconc. Factor (BCF)	1.07	pH 1 25 deg C (	1)
Bioconc. Factor (BCF)	6.15	1 1	1)
Bioconc. Factor (BCF)	12.10		1)
Bioconc. Factor (BCF)	13.40	<u> </u>	1)
Bioconc. Factor (BCF)	13.55	!=	1)
Bioconc. Factor (BCF)	13.56	, ,	1)
Bioconc. Factor (BCF)	13.56	12	1)
Bioconc. Factor (BCF)	13.52	,-	1)
Bioconc. Factor (BCF)	13.11		1)
Bioconc. Factor (BCF)	10.08		1)
Density (DEN)	1.290+/-0.06 g/cm**3	,	1)
Freely Rotatable Bonds (FRB)	2	•	1)
H acceptors (HAC)	6	•	1)
H donors (HD)	2	!	1)
Hydrogen Donors/Acceptors Sum (HDAS)	8 	(.	1)
Koc (KOC)	17.75	рн 1 25 deg C (:	1)
Koc (KOC)	101.91	pH 2 25 deg C (	1)
Koc (KOC)	200.58		1)
Koc (KOC)	222.17		1)
Koc (KOC)	224.59		1)
Koc (KOC)	224.82		1)
Koc (KOC)	224.78	рн 7 25 deg C (:	1)
Koc (KOC)	224.08	рн 8 25 deg C (:	1)
Koc (KOC)	217.33	рн 9 25 deg C (	1)
Koc (KOC)	167.13	pH 10 25 deg C (	1)
logD (LOGD)	0.69	рн 1 25 deg C (	1)
logD (LOGD)	1.45	pH 2 25 deg C (	1)
logD (LOGD)	1.74	pH 3 25 deg C (	1)
logD (LOGD)	1.79		1)
logD (LOGD)	1.79		1)
logD (LOGD)	1.79		1)
logD (LOGD)	1.79		1)

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logD (LOGD)
                               1.79
                                                       pH 8
                                                             25 deg C
                                                                          (1)
logD (LOGD)
                                1.78
                                                       pH 9 25 deg C
                                                                          (1)
logD (LOGD)
                                1.66
                                                       pH 10 25 deg C
                                                                          (1)
                                1.793+/-0.598
                                                       25 deg C
logP (LOGP)
                                                                          (1)
                                                       25 deg C
                                                                          (1)
Mass Intrinsic Solubility
                                0.12 \, \text{g/L}
 (ISLB.MASS)
                               1.5 g/L
                                                       pH 1
                                                              25 deg C
                                                                          (1)
Mass Solubility (SLB.MASS)
                                0.27 g/L
Mass Solubility (SLB.MASS)
                                                       pH 2
                                                              25 deg C
                                                                          (1)
                                                       pH 3
Mass Solubility (SLB.MASS)
                                0.14 \text{ g/L}
                                                              25 deg C
                                                                          (1)
                                                       pH 4
Mass Solubility (SLB.MASS)
                                0.12 \, g/L
                                                              25 deg C
                                                                          (1)
                                                       pH 5
Mass Solubility (SLB.MASS)
                                0.12 g/L
                                                              25 deg C
                                                                          (1)
                                                      |pH 6
Mass Solubility (SLB.MASS)
                                0.12 g/L
                                                              25 deg C
                                                                          (1)
                                                      |pH 7
Mass Solubility (SLB.MASS)
                                0.12 g/L
                                                              25 deg C
                                                                          (1)
                                                      | pH 8
Mass Solubility (SLB.MASS)
                                0.12 g/L
                                                              25 deg C
                                                                          (1)
                                                       |pH 9 25 deg C
Mass Solubility (SLB.MASS)
                                0.13 g/L
                                                                          (1)
                                                       |pH 10 25 deg C
Mass Solubility (SLB.MASS)
                                0.16 g/L
                                                                          (1)
Mass Solubility (SLB.MASS)
                                0.12 \, g/L
                                                       |Unbuffered Water
                                                                         (1)
                                                       pH 6.81
                                                       25 deg C
                                                       25 deg C
Molar Intrinsic Solubility
                                0.00042 mol/L
                                                                          (1)
 (ISLB.MOL)
Molar Solubility (SLB.MOL)
                                0.0054 mol/L
                                                       pH 1
                                                             25 deg C
                                                                          (1)
                                                       pH 2
Molar Solubility (SLB.MOL)
                                0.00094 mol/L
                                                             25 deg C
                                                                          (1)
                                                       pH 3
Molar Solubility (SLB.MOL)
                                0.00048 mol/L
                                                              25 deg C
                                                                          (1)
                                                       pH 4
Molar Solubility (SLB.MOL)
                                0.00043 mol/L
                                                              25 deg C
                                                                          (1)
Molar Solubility (SLB.MOL)
                                0.00042 mol/L
                                                       pH 5
                                                              25 deg C
                                                                          (1)
Molar Solubility (SLB.MOL)
                                0.00042 mol/L
                                                       pH 6
                                                              25 deg C
                                                                          (1)
                                                       pH 7
Molar Solubility (SLB.MOL)
                                0.00042 mol/L
                                                              25 deg C
                                                                          (1)
Molar Solubility (SLB.MOL)
                                0.00043 \text{ mol/L}
                                                       8 Hq
                                                              25 deg C
                                                                          (1)
Molar Solubility (SLB.MOL)
                                0.00044 mol/L
                                                       pH 9 25 deg C
                                                                          (1)
Molar Solubility (SLB.MOL)
                                0.00057 mol/L
                                                       pH 10 25 deg C
                                                                          (1)
                                                       Unbuffered Water
Molar Solubility (SLB.MOL)
                                0.00042 mol/L
                                                                         (1)
                                                       pH 6.81
                                                       25 deg C
Molar Volume (MVOL)
                                220.3+/-3.0 cm**3/mol|20 deg C
                                                                          (1)
                                                       760 Torr
                                284.31
                                                                          (1)
Molecular Weight (MW)
                                10.46+/-0.70
                                                       Most Acidic
                                                                          (1)
pKa (PKA)
                                                       25 deg C
                                2.08+/-0.50
                                                       Most Basic
                                                                          (1)
pKa (PKA)
                                                       25 deg C
Polar Surface Area (PSA)
                               83.98 A**2
                                                                          (1)
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(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.19 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

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L5 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
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RN 280768-70-9 REGISTRY

ED Entered STN: 27 Jul 2000

CN 4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phe nyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H21 Cl N6 O2

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

# Ring System Data

Analysis EA	Sequence ES	the Rings SZ	Ring System Formula RF	Identifier RID	Count
C6	C6   NC5	6	C6	46.150.18 46.156.1	

# Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION   NOTE
Bioconc. Factor (BCF) Bioconc. Factor (BCF) Bioconc. Factor (BCF) Bioconc. Factor (BCF)	1.0   1.0   1.0   1.0	pH 1     25 deg C     (1)       pH 2     25 deg C     (1)       pH 3     25 deg C     (1)       pH 4     25 deg C     (1)
Bioconc. Factor (BCF) Bioconc. Factor (BCF)	1.0	pH 5 25 deg C (1) pH 6 25 deg C (1)
Bioconc. Factor (BCF)	1.0  1.0	pH 7 25 deg C (1)
Bioconc. Factor (BCF) Bioconc. Factor (BCF)	1.0	pH 9 25 deg C (1)
Bioconc. Factor (BCF) Density (DEN)	1.70  1.405+/-0.06 g/cm**3	pH 10 25 deg C   (1)   760 Torr   (1)
Freely Rotatable Bonds (FRB) H acceptors (HAC)	<del>4</del>   8	(1)
H donors (HD) Hydrogen Donors/Acceptors Sum (HDAS)	2  10 	(1)
Koc (KOC)	1.73  1.75	pH 1 25 deg C   (1)  pH 2 25 deg C   (1)
Koc (KOC) Koc (KOC)	1.76	pH 3 25 deg C (1)
Koc (KOC)	1.76	pH 4 25 deg C (1)
Koc (KOC)	1.76  1.76	pH 5 25 deg C   (1)  pH 6 25 deg C   (1)
Koc (KOC) Koc (KOC)	1.83	pH 6 25 deg C  (1)  pH 7 25 deg C  (1)
Koc (KOC)	2.47	pH 8 25 deg C (1)
Koc (KOC)	7.46	pH 9 25 deg C (1)
Koc (KOC)	19.72	pH 10 25 deg C (1)
logD (LOGD) logD (LOGD)	0.01  0.01	pH 1 25 deg C  (1)  pH 2 25 deg C  (1)
logD (LOGD)	0.01	pH 3 25 deg C (1)
logD (LOGD)	0.01	pH 4 25 deg C (1)
logD (LOGD)	0.01	pH 5 25 deg C (1)
logD (LOGD)	0.02	рн 6 25 deg C (1)
logD (LOGD)	0.03	pH 7 25 deg C (1)
logD (LOGD)	0.16	рн 8 25 deg C (1)
logD (LOGD)	0.64	pH 9 25 deg C (1)
logD (LOGD)	1.06	pH 10 25 deg C (1)
logP (LOGP)	2.514+/-0.646	25 deg C   (1)
Mass Intrinsic Solubility (ISLB.MASS)	0.011 g/L 	25 deg C
Mass Solubility (SLB.MASS)	3.7 g/L	pH 1 25 deg C (1)
	3.6 g/L	pH 2 25 deg C (1)
Mass Solubility (SLB.MASS)	3.6 g/L	pH 3 25 deg C  (1)

```
pH 4
                                                            25 deg C
Mass Solubility (SLB.MASS)
                              3.6 \text{ g/L}
                                                                        (1)
                                                      pH 5
                                                            25 deg C
                                                                         (1)
Mass Solubility (SLB.MASS)
                               3.6 g/L
                                                      рн 6
Mass Solubility (SLB.MASS)
                               3.4 g/L
                                                            25 deg C
                                                                         (1)
                                                      pH 7
Mass Solubility (SLB.MASS)
                               2.3 g/L
                                                             25 deg C
                                                                         (1)
                                                      pH 8
                                                            25 deg C
                                                                         (1)
Mass Solubility (SLB.MASS)
                               0.57 g/L
                                                      |pH 9 25 deg C
                                                                         (1)
Mass Solubility (SLB.MASS)
                               0.079 g/L
                               0.026 g/L
                                                      |pH 10 25 deg C
                                                                         (1)
Mass Solubility (SLB.MASS)
                                                      |Unbuffered Water | (1)
Mass Solubility (SLB.MASS)
                               0.035 \text{ g/L}
                                                      pH 9.57
                                                      |25 deg C
                               0.000026 mol/L
                                                      25 deg C
Molar Intrinsic Solubility
                                                                         (1)
 (ISLB.MOL)
                                                      |pH 1 25 deg C
                                                                         (1)
Molar Solubility (SLB.MOL)
                               0.0084 \text{ mol/L}
                               0.0083 mol/L
                                                      |pH 2 25 deg C
                                                                         (1)
Molar Solubility (SLB.MOL)
Molar Solubility (SLB.MOL)
                               0.0083 mol/L
                                                      pH 3
                                                            25 deg C
                                                                         (1)
                               0.0083 mol/L
                                                      pH 4
                                                            25 deg C
                                                                         (1)
Molar Solubility (SLB.MOL)
                                                      pH 5
                               0.0082 mol/L
                                                            25 deg C
                                                                         (1)
Molar Solubility (SLB.MOL)
                                                      |pH 6 25 deg C
Molar Solubility (SLB.MOL)
                               0.0078 mol/L
                                                                         (1)
                                                      pH 7 25 deg C
                               0.0053 mol/L
                                                                         (1)
Molar Solubility (SLB.MOL)
                                                      pH 8 25 deg C
                                                                         (1)
Molar Solubility (SLB.MOL)
                               0.0013 mol/L
                                                      pH 9 25 deg C
                               0.00018 mol/L
                                                                         (1)
Molar Solubility (SLB.MOL)
                                                      |pH 10 25 deg C
                                                                         (1)
Molar Solubility (SLB.MOL)
                               0.000059 mol/L
                                                      |Unbuffered Water|(1)
                               0.000080 mol/L
Molar Solubility (SLB.MOL)
                                                      pH 9.57
                                                      25 deg C
                                                                         (1)
                               |310.7+/-3.0 cm**3/mol|20 deg C
Molar Volume (MVOL)
                                                      760 Torr
                                                                         (1)
Molecular Weight (MW)
                               436.89
                                                                         (1)
                               9.58 + / - 0.70
                                                      Most Acidic
pKa (PKA)
                                                      25 deg C
                               10.88+/-0.10
                                                      Most Basic
                                                                         (1)
pKa (PKA)
                                                      25 deg C
Polar Surface Area (PSA)
                               100.11 A**2
                                                                         (1)
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(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

133:89437 CA

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Preparation of heteroaryl-substituted aromatic amides as factor Xa
    Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman;
    Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven
    Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine
    Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez,
    Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald
     Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton;
    Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
    Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
    PCT Int. Appl., 403 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
IC
     ICM C07D401-14
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C07D401-12; C07D417-14; C07D409-14; C07D405-14; C07D213-74;

A61K031-395; A61K031-435; A61K031-495; A61P007-02; C07D401-14; C07D213-00; C07D213-00; C07D211-00

27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 28, 63

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE
PI WO 2000039118 A1 20000706 WO 1999-US29946 19991215

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,

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280769-01-9P

GI

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280768-80-1P

280768-85-6P

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280768-95-8P

280769-00-8P

are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un) substituted at the 5-position, 3-pyridinyl (un) substituted at the 6-position, 2-pyrimidinyl (un) substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; <math>Q2 =(un) substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day. arom amide heteroaryl prepn formulation factor Xa inhibitor anticoagulant ST IT Anticoagulants (preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors) 280769-23-5P 280769-24-6P 280769-16-6P 280769-22-4P IT 280769-11-1P 280769-68-8P 280769-83-7P 280770-51-6P 280769-46-2P 280769-59-7P 280770-79-8P 280770-91-4P 280770-59-4P 280770-66-3P 280770-52-7P 280771-19-9P 280771-47-3P 280771-49-5P 280770-93-6P 280770-95-8P 280771-53-1P 280771-55-3P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors) 280768-69-6P 280768-66-3P 280768-67-4P 280768-68-5P

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                       98-01-1, Furan-2-carboxaldehyde, reactions
2-Ethylbutyraldehyde
98-74-8, 4-Nitrobenzenesulfonyl chloride
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107-13-1, 2-Propenenitrile, reactions
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Cyclopentanone
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4-Methoxybenzaldehyde, reactions
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        (preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)
              THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
        6
(1) Beight Douglas Wade; WO 9900121 A 1999 CAPLUS
(2) Beight Douglas Wade; WO 9900128 A 1999 CAPLUS
(3) Berlex Lab; WO 9628427 A 1996 CAPLUS
(4) Katakura; EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY CHIMICA THERAPEUTICA
    1995, V30(5), P387 CAPLUS
(5) Kunitada, S; CURRENT PHARMACEUTICAL DESIGN 1996, V2(5), P6
(6) Schering Ag; WO 9932477 A 1999 CAPLUS
     ANSWER 4 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
     267891-53-2 REGISTRY
     Entered STN: 02 Jun 2000
     Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI)
     (CA INDEX NAME)
     3D CONCORD
     C21 H16 Cl N5 O
     CA
     STN Files:
                  CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
       Roles from patents: BIOL (Biological study); PREP (Preparation); USES
RL.P
       (Uses)
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Ring System Data

IT

L5

RN

ED

CN

FS

MF

SR

LC

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
========	-========	+=======-	}=========	-========	+=======
C6	C6	6	C6	46.150.18	1
C5N	NC5	6	C5N	46.156.30	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.47	1

# Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF) Density (DEN) Freely Rotatable Bonds (FRB) H acceptors (HAC) H donors (HD) Hydrogen Donors/Acceptors Sum (HDAS)	1.0 1.12 6.75 45.32 116.61 136.68 122.15 55.70 10.63 1.421+/-0.06 g/cm**3   4	PH 1 25 deg C   PH 2 25 deg C   PH 3 25 deg C   PH 4 25 deg C   PH 5 25 deg C   PH 6 25 deg C   PH 7 25 deg C   PH 8 25 deg C   PH 9 25 deg C   PH 10 25 deg	(1) (1) (1) (1) (1) (1) (1) (1) (1) (1)
Koc (KOC) LogD (LOGD)	1.64 3.48 8.07 48.75 327.37 842.43 987.39 882.47 402.41 76.78 0.42 0.74 1.11 1.89 2.72 3.13 3.20 3.15 2.81 2.09 3.463+/-0.615 0.0036 g/L	pH       1       25 deg C         pH       2       25 deg C         pH       3       25 deg C         pH       4       25 deg C         pH       5       25 deg C         pH       6       25 deg C         pH       7       25 deg C         pH       9       25 deg C         pH       1       25 deg C         pH       1       25 deg C         pH       2       25 deg C         pH       4       25 deg C         pH       5       25 deg C         pH       6       25 deg C         pH       7       25 deg C         pH       9       25 deg C         pH       10       25 deg C	(1) (1) (1) (1) (1) (1) (1) (1) (1) (1)
(ISLB.MASS) Mass Solubility (SLB.MASS)	:	рн 4 25 deg C рн 5 25 deg C	  (1)  (1)  (1)  (1)  (1)

```
pH 7
                              0.0062 g/L
                                                           25 deg C
                                                                       (1)
Mass Solubility (SLB.MASS)
                               0.0070 g/L
                                                     8 Hg
                                                           25 deg C
                                                                       (1)
Mass Solubility (SLB.MASS)
Mass Solubility (SLB.MASS)
                               0.015 g/L
                                                     pH 9 25 deg C
                                                                       (1)
                               0.082 g/L
Mass Solubility (SLB.MASS)
                                                     |pH 10 25 deg C
                                                                       (1)
                               0.0062 g/L
                                                     |Unbuffered Water|(1)
Mass Solubility (SLB.MASS)
                                                     pH 7.05
                                                     25 deg C
                               0.0000093 mol/L
                                                     25 deg C
                                                                       (1)
Molar Intrinsic Solubility
 (ISLB.MOL)
                               0.010 mol/L
                                                     |pH 1 25 deg C
Molar Solubility (SLB.MOL)
                                                                       (1)
                                                     pH 2
Molar Solubility (SLB.MOL)
                               0.0048 mol/L
                                                           25 deg C
                                                                       (1)
Molar Solubility (SLB.MOL)
                                                     pH 3
                               0.0020 mol/L
                                                           25 deg C
                                                                       (1)
Molar Solubility (SLB.MOL)
                               0.00032 mol/L
                                                     |pH 4 25 deg C
                                                                       (1)
                                                     pH 5
Molar Solubility (SLB.MOL)
                               0.000047 mol/L
                                                           25 deg C
                                                                       (1)
                               0.000018 mol/L
                                                     pH 6 25 deg C
                                                                       (1)
Molar Solubility (SLB.MOL)
Molar Solubility (SLB.MOL)
                               0.000016 mol/L
                                                     pH 7
                                                           25 deg C
                                                                       (1)
Molar Solubility (SLB.MOL)
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                                                     |pH 8 25 deg C
                                                                       (1)
                               0.000039 mol/L
                                                     pH 9 25 deg C
                                                                       (1)
Molar Solubility (SLB.MOL)
                               0.00021 mol/L
                                                     pH 10 25 deg C
                                                                       (1)
Molar Solubility (SLB.MOL)
Molar Solubility (SLB.MOL)
                              0.000016 mol/L
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                                                     pH 7.05
                                                     25 deg C
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                                                                       (1)
Molar Volume (MVOL)
                                                     760 Torr
Molecular Weight (MW)
                               389.84
                                                                       (1)
                               8.54+/-0.43
                                                     Most Acidic
                                                                       (1) (2)
pKa (PKA)
                                                     25 deg C
                               5.34+/-0.10
                                                     Most Basic
                                                                       (1) (2)
pKa (PKA)
                                                     25 deg C
                              79.80 A**2
Polar Surface Area (PSA)
                                                                       (1)
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This substance may exist in multiple tautomeric forms. The property values in this table are calculated based upon the displayed form and may therefore differ from experimental values based on the actual tautomeric ratio at equilibrium.

- (1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)
- (2) A significant difference may occur between experimental and calculated values.

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

FAN.CNT 2

Section cross-reference(s): 1

```
132:334364 CA
ΑN
ΤI
     Preparation of anthranilic acid amides as vascular endothelial growth
     factor receptor inhibitors.
    Huth, Andreas; Seidelmann, Dieter; Thierauch, Karl-Heinz; Bold, Guido;
ΙN
     Manley, Paul William; Furet, Pascal; Wood, Jeanette Marjorie; Mestan,
    Jurgen; Bruggen, Jose; Ferrari, Stefano; Kruger, Martin; Ottow, Eckhard;
     Menrad, Andreas; Schirner, Michael
    Schering Aktiengesellschaft, Germany; Novartis Aktiengesellschaft
PA
SO
     PCT Int. Appl., 96 pp.
     CODEN: PIXXD2
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     Patent
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     German
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    PATENT NO.
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    WO 1999-EP8478
                      19991109
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PΤ

GI

Title compds. [I; A = NR2; W = O, S, H2, NR8; Z = NR10, N, NR10(CH2)q, AΒ alkyl, etc.; q = 1-6; AZR1 = tetrahydroisoquinolinyl, indazolyl, 5-chloroindolyl, etc.; R1 = (substituted) aryl, heteroaryl; R2 = H, alkyl; R3 = (substituted) mono- or bicyclic aryl, heteroaryl; R4-R7 = H, halo, (substituted) alkoxy, alkyl, carboxyalkyl; R5R6 = dioxetanyl; R8, R10 = H, alkyl]. Thus, Me N-(4-pyridylmethyl)anthranilate (preparation given) was stirred with Ph(CH2)3NH2 and Me3Al were stirred in PhMe to give N-(3-phenylprop-1-yl)-N2-(4-pyridylmethyl)anthranilamide. The latter inhibited VEGFR I with IC50 =  $0.05 \mu M$ .

anthranilamide prepn VEGF receptor inhibitor; angiogenesis inhibitor stanthranilamide; vascular endothelial growth factor receptor inhibitor prepn anthranilamide

Blood vessel, neoplasm IT

(angiofibroma, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Medical goods

(catheters, antithrombogenic; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Kidney, disease

(diabetic nephropathy, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

Vascular endothelial growth factor receptors IT RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process) (gene KDR, inhibitors; preparation of anthranilic acid amides as VEGF

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receptor inhibitors)
    Vascular endothelial growth factor receptors
IT
    RL: BPR (Biological process); BSU (Biological study, unclassified); MSC
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        (glomerulonephritis, treatment; preparation of anthranilic acid amides as
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    Blood vessel, neoplasm
TT
        (hemangioma, treatment; preparation of anthranilic acid amides as VEGF
       receptor inhibitors)
    Nerve, disease
IT
        (injury, treatment; preparation of anthranilic acid amides as VEGF receptor
        inhibitors)
    Blood vessel, disease
IT
        (microangiopathy, treatment of thrombotic microangiopathy; preparation of
       anthranilic acid amides as VEGF receptor inhibitors)
    Kidney, disease
IT
        (nephrosclerosis, treatment of malignant nephrosclerosis; preparation of
       anthranilic acid amides as VEGF receptor inhibitors)
    Angiogenesis inhibitors
IT
    Antiarteriosclerotics
    Antiarthritics
    Antitumor agents
        (preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT
    Medical goods
        (stents, opening maintenance; preparation of anthranilic acid amides as VEGF
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     Transplant rejection
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(Uses)

(preparation of anthranilic acid amides as VEGF receptor inhibitors) IT 104-86-9, 4-Chlorobenzylamine 118-48-9, Isatoic anhydride 123-11-5, 4-Methoxybenzaldehyde, reactions 134-20-3, Methyl anthranilate 9, 2-Phenylpropylamine 635-21-2, 5-Chloroanthranilic acid 872 582-22-872-85-5, 19335-11-6, 5-Aminoindazole Pyridine-4-carboxaldehyde 101066-61-9, 2-Chloro-4-pyridinecarboxaldehyde 267891-90-7 267891-89-4 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of anthranilic acid amides as VEGF receptor inhibitors) IT 16512-74-6P 267891-86-1P 267891-87-2P 267891-88-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of anthranilic acid amides as VEGF receptor inhibitors) L5 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN 267891-24-7 REGISTRY Entered STN: 02 Jun 2000 ED

RN

Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) CN

(CA INDEX NAME)

3D CONCORD FS

C17 H14 Cl N5 O MF

SR CA

CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL LCSTN Files:

DT.CA CAplus document type: Patent

Roles from patents: BIOL (Biological study); PREP (Preparation); USES RL.P (Uses)

## Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
========	H=======	+======+	+========	+=======-	+========
C6	C6	6	C6	46.150.18	1
C5N	NC5	6	C5N	46.156.30	1
C4N2	NCNC3	6	C4N2	46.195.39	1

### Predicted Properties (PPROP)

PROPERTY	(CODE)	VALUE		COI	MI.	CION		NOTE
=======================================	==========	+======================================	+===	===	===	====	===	+====
Bioconc. Factor	(BCF)	1.0	pН	1	25	deg	C	(1)
Bioconc. Factor	(BCF)	1.0	pН	2	25	deg	С	(1)
Bioconc. Factor	(BCF)	1.0	рн	3	25	deg	С	(1)
Bioconc. Factor	(BCF)	1.0	рH	4	25	deg	С	(1)
Bioconc. Factor	(BCF)	6.52	рН	5	25	deg	C	(1)
Bioconc. Factor	(BCF)	16.71	рн	6	25	deg	C	(1)
Bioconc. Factor	(BCF)	19.82	pН	7	25	deg	С	(1)
Bioconc. Factor	(BCF)	20.02	рН	8	25	deg	С	(1)

Bioconc. Factor (BCF) Bioconc. Factor (BCF) Density (DEN) Freely Rotatable Bonds (FRB) H acceptors (HAC) H donors (HD) Hydrogen Donors/Acceptors Sum (HDAS)	18.47   10.34   1.415+/-0.06 g/cm**3   4   6   2   8	рн 9 25 deg C рн 10 25 deg C 760 Torr	(1) (1) (1) (1) (1) (1)
(HDAS) Koc (KOC) LogD (LOGD) LogP (LOGP) Mass Intrinsic Solubility	1.0  1.05  2.34  14.35  96.41  247.20  293.14  296.15  273.17  152.97  -0.60  -0.43  -0.09  0.70  1.53  1.94  2.01  2.02  1.98  1.73  2.022+/-0.612  0.054 g/L	рн 8 25 deg C рн 9 25 deg C рн 10 25 deg C рн 1 25 deg C	(1) (1) (1) (1) (1) (1) (1) (1) (1) (1)
(ISLB.MASS) Mass Solubility (SLB.MASS)	23 g/L	  pH 1 25 deg C	(1) (1) (1) (1) (1) (1) (1) (1) (1)
(ISLB.MOL) Molar Solubility (SLB.MOL)	0.046 mol/L  0.021 mol/L  0.0034 mol/L	PH 2 25 deg C PH 3 25 deg C PH 4 25 deg C PH 5 25 deg C PH 6 25 deg C PH 7 25 deg C PH 8 25 deg C	(1) (1) (1) (1) (1) (1) (1) (1) (1)
Molar Volume (MVOL)  Molecular Weight (MW) pKa (PKA)	240.0+/-3.0 cm**3/mol 339.78 10.01+/-0.70		(1) (1) (1)
pKa (PKA)	5.33+/-0.10	25 deg C  Most Basic	(1)
Polar Surface Area (PSA)	79.80 A**2	25 deg C	(1)

This substance may exist in multiple tautomeric forms. The property values in

this table are calculated based upon the displayed form and may therefore differ from experimental values based on the actual tautomeric ratio at equilibrium.

Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 (1)

((C) 1994-2006 ACD/Labs) See HELP PROPERTIES for information about property data sources in REGISTRY. 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE) REFERENCE 1 AN 132:334364 CA Preparation of anthranilic acid amides as vascular endothelial growth ΤI factor receptor inhibitors. IN Huth, Andreas; Seidelmann, Dieter; Thierauch, Karl-Heinz; Bold, Guido; Manley, Paul William; Furet, Pascal; Wood, Jeanette Marjorie; Mestan, Jurgen; Bruggen, Jose; Ferrari, Stefano; Kruger, Martin; Ottow, Eckhard; Menrad, Andreas; Schirner, Michael Schering Aktiengesellschaft, Germany; Novartis Aktiengesellschaft PA PCT Int. Appl., 96 pp. SO CODEN: PIXXD2 DTPatent German LA ICM C07D213-38 IC ICS C07D409-12; C07D401-12; C07D213-40; C07D413-12; C07D401-12; C07D401-12; C07C237-30; C07D213-61; C07D417-12; C07D401-12; C07D401-12; C07D401-14; C07D401-12; C07D405-12; C07D417-12; C07D405-12; C07D265-26 CC27-16 (Heterocyclic Compounds (One Hetero Atom)) Section cross-reference(s): 1 FAN.CNT 2 PATENT NO. KIND DATE APPLICATION NO. DATE --------------WO 2000027819 A2 WO 1999-EP8478 20000518 19991109 PΙ 20000817 WO 2000027819 A3 W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG DE 19910396 A1 20000907 DE 1999-19910396 19990303 DE 19910396 C2 20011213 CA 1999-2350208 19991109 CA 2350208 AΑ 20000518 BR 9915553 Α 20010814 BR 1999-15553 19991109 EP 1129074 A2 20010905 EP 1999-953967 19991109

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
        IE, SI, LT, LV, FI, RO
                       20020521
                                      TR 2001-20010130719991109
TR 200101307
                  T2
                                      JP 2000-580999
                                                       19991109
JP 2002529452
                  T2
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EE 200100258
                  Α
                       20021216
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AU 771180
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                                                       20010507
                  Α
                       20010710
BG 105588
                                      BG 2001-105588
                                                       20010611
                  Α
                       20020430
HK 1041882
                 A1
                       20050318
                                      HK 2002-103628
                                                       20020514
```

PRAI GB 1998-24579 19981110 DE 1999-19910396 19990303 WO 1999-EP8478 19991109

AB Title compds. [I; A = NR2; W = O, S, H2, NR8; Z = NR10, N, NR10(CH2)q, alkyl, etc.; q = 1-6; AZR1 = tetrahydroisoquinolinyl, indazolyl, 5-chloroindolyl, etc.; R1 = (substituted) aryl, heteroaryl; R2 = H, alkyl; R3 = (substituted) mono- or bicyclic aryl, heteroaryl; R4-R7 = H, halo, (substituted) alkoxy, alkyl, carboxyalkyl; R5R6 = dioxetanyl; R8, R10 = H, alkyl]. Thus, Me N-(4-pyridylmethyl)anthranilate (preparation given) was stirred with Ph(CH2)3NH2 and Me3Al were stirred in PhMe to give N-(3-phenylprop-1-yl)-N2-(4-pyridylmethyl)anthranilamide. The latter inhibited VEGFR I with IC50 = 0.05 μM.

ST anthranilamide prepn VEGF receptor inhibitor; angiogenesis inhibitor anthranilamide; vascular endothelial growth factor receptor inhibitor prepn anthranilamide

IT Blood vessel, neoplasm

(angiofibroma, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Medical goods

IT

IT

(catheters, antithrombogenic; preparation of anthranilic acid amides as VEGF receptor inhibitors)

Kidney, disease

(diabetic nephropathy, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Vascular endothelial growth factor receptors

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(gene KDR, inhibitors; preparation of anthranilic acid amides as VEGF receptor inhibitors)

Vascular endothelial growth factor receptors

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(gene flt 1, inhibitors; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Kidney, disease

(glomerulonephritis, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Blood vessel, neoplasm

(hemangioma, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Nerve, disease

(injury, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Blood vessel, disease

(microangiopathy, treatment of thrombotic microangiopathy; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Kidney, disease

(nephrosclerosis, treatment of malignant nephrosclerosis; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Angiogenesis inhibitors

Antiarteriosclerotics

Antiarthritics

Antitumor agents

(preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Medical goods

(stents, opening maintenance; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Cirrhosis

Eye, disease

Kidney, disease

Psoriasis

```
(treatment; preparation of anthranilic acid amides as VEGF receptor
       inhibitors)
ΙT
    267891-62-3P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (preparation of anthranilic acid amides as VEGF receptor inhibitors)
                                                267891-07-6P
IT
                   267891-05-4P
                                 267891-06-5P
                                                               267891-08-7P
    267891-04-3P
                                                               267891-13-4P
                                 267891-11-2P
                                                267891-12-3P
    267891-09-8P
                   267891-10-1P
                                                               267891-18-9P
                                 267891-16-7P
                                                267891-17-8P
                   267891-15-6P
    267891-14-5P
                   267891-20-3P
                                 267891-21-4P
                                                267891-22-5P
                                                               267891-23-6P
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                                 267891-26-9P
                                                267891-27-0P
                                                               267891-28-1P
                   267891-25-8P
    267891-24-7P
                   267891-30-5P
                                 267891-31-6P
                                                267891-32-7P
                                                               267891-33-8P
    267891-29-2P
                                                267891-37-2P
                                                               267891-38-3P
    267891-34-9P
                   267891-35-0P
                                 267891-36-1P
                                                267891-42-9P
                                                               267891-43-0P
                   267891-40-7P
                                 267891-41-8P
    267891-39-4P
                                                               267891-48-5P
                                                267891-47-4P
                   267891-45-2P
                                 267891-46-3P
    267891-44-1P
                                 267891-51-0P
                                                               267891-53-2P
                   267891-50-9P
                                                267891-52-1P
    267891-49-6P
                                                               267891-58-7P
                                                267891-57-6P
    267891-54-3P
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                                 267891-56-5P
                                                               267891-64-5P
                                 267891-61-2P
                                                267891-63-4P
    267891-59-8P
                   267891-60-1P
                                                267891-68-9P
                                                               267891-69-0P
                                 267891-67-8P
    267891-65-6P
                   267891-66-7P
                                                               267891-75-8P
                                 267891-73-6P
                                                267891-74-7P
                   267891-72-5P
    267891-70-3P
                                                267891-79-2P
                                                               267891-80-5P
                                 267891-78-1P
                   267891-77-0P
    267891-76-9P
                                 267891-83-8P
                                                267891-84-9P
                                                               267891-85-0P
    267891-81-6P
                   267891-82-7P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of anthranilic acid amides as VEGF receptor inhibitors)
                                                           267891-95-2
                               267891-93-0
                                             267891-94-1
IT
    267891-91-8
                  267891-92-9
                                267891-98-5
                                             267891-99-6
                                                           267892-00-2
     267891-96-3
                  267891-97-4
                               267892-03-5
                                                           267892-05-7
     267892-01-3
                  267892-02-4
                                             267892-04-6
                                                           267892-12-6
                                             267892-11-5
     267892-06-8
                  267892-07-9
                               267892-09-1
                  267892-14-8 267892-15-9
     267892-13-7
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (preparation of anthranilic acid amides as VEGF receptor inhibitors)
     104-86-9, 4-Chlorobenzylamine 118-48-9, Isatoic anhydride
                                                                 123-11-5,
IT
     4-Methoxybenzaldehyde, reactions 134-20-3, Methyl anthranilate
                                                                      582-22-
     9, 2-Phenylpropylamine 635-21-2, 5-Chloroanthranilic acid
                                                                872-85-5,
     Pyridine-4-carboxaldehyde
                               19335-11-6, 5-Aminoindazole
                                                            101066-61-9,
     2-Chloro-4-pyridinecarboxaldehyde 267891-89-4
                                                     267891-90-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of anthranilic acid amides as VEGF receptor inhibitors)
                                267891-87-2P
                                               267891-88-3P
                  267891-86-1P
IT
     16512-74-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of anthranilic acid amides as VEGF receptor inhibitors)
    ANSWER 6 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
L5
     180206-29-5 REGISTRY
RN
     Entered STN: 29 Aug 1996
ED
     Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI)
CN
    NAME)
     3D CONCORD
FS
     C32 H27 N3 O4
MF
SR
     CA
LC
     STN Files:
                 CA, CAPLUS
DT.CA CAplus document type: Patent
      Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
RL.P
       (Reactant or reagent)
Ring System Data
Elemental | Size of | Ring System |
                                            Ring
                                         Identifier Occurrence
Analysis | Sequence | the Rings |
                               Formula
         | ES
                     SZ
                                RF
                                           RID
                                                  Count
______+
                       |C6
                                  46.150.18 4
```

Transplant rejection

$$\begin{array}{c|c}
 & O & O - CH_2 - Ph \\
 & O & O - CH_2 - Ph \\
 & O - CH_2 - Ph \\
 & O - CH_2 - Ph
\end{array}$$

## Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	8607.26	рн 1 25 deg C	(1)
Bioconc. Factor (BCF)	10515.24	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	10753.82	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	10778.27	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	10780.63	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	10780.01	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	10771.36	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	10685.44	рн 8 25 deg C	(1)
Bioconc. Factor (BCF)	9896.65	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	5715.35	pH 10 25 deg C	(1)
Density (DEN)	1.265+/-0.06 g/cm**3	760 Torr	(1)
Freely Rotatable Bonds (FRB)	10		(1)
H acceptors (HAC)	7	]	(1)
H donors (HD)	1	]	(1)
Hydrogen Donors/Acceptors Sum	8		(1)
(HDAS)		- 1 2 de - C	/11
Koc (KOC)	21384.27	pH 1 25 deg C	(1)
Koc (KOC)	26124.53	pH 2 25 deg C	(1)
Koc (KOC)	26717.24	pH 3 25 deg C	(1)
Koc (KOC)	26777.98	pH 4 25 deg C   pH 5 25 deg C	(1)
Koc (KOC)	26783.86  26782.33	pH 6 25 deg C	(1)
Koc (KOC) Koc (KOC)	26760.84	pH 7 25 deg C	(1)
Koc (KOC)	26547.35	pH 8 25 deg C	(1)
Koc (KOC)	24587.68	pH 9 25 deg C	(1)
Koc (KOC)	14199.46	pH 10 25 deg C	(1)
logD (LOGD)	5.51	pH 1 25 deg C	(1)
logD (LOGD)	5.60	pH 2 25 deg C	(1)
logD (LOGD)	5.61	pH 3 25 deg C	(1)
logD (LOGD)	5.61	pH 4 25 deg C	(1)
logD (LOGD)	5.61	pH 5 25 deg C	(1)
logD (LOGD)	5.61	рн 6 25 deg C	(1)
logD (LOGD)	5.61	pH 7 25 deg C	(1)
logD (LOGD)	5.60	pH 8 25 deg C	(1)
logD (LOGD)	5.57	pH 9 25 deg C	(1)
logD (LOGD)	5.33	pH 10 25 deg C	(1)
logP (LOGP)	5.610+/-0.611	25 deg C	(1)
Mass Intrinsic Solubility	0.00016 g/L	25 deg C	(1)
(ISLB.MASS)			1,5
Mass Solubility (SLB.MASS)	0.00020 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 4 25 deg C   pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L  0.00016 g/L	рн 5 25 deg C рн 6 25 deg C	(1)
Mass Solubility (SLB.MASS) Mass Solubility (SLB.MASS)	0.00016 g/L  0.00016 g/L	ph 6 25 deg C	(1)
Mass Solubility (SLB.MASS) Mass Solubility (SLB.MASS)	0.00016 g/L  0.00016 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)  Mass Solubility (SLB.MASS)	0.00016 g/L 0.00017 g/L	рн 8 25 deg C	(1)
mass borubility (bub.MASS)	10.0001/ 9/1	15 2 22 469 6	\ _ /

Mass Solubility (SLB.MASS)	0.00030 g/L	pH 10 25 deg C Unbuffered Water	•
Mass Solubility (SLB.MASS)	0.00016 g/L 	pH 7.00	(
		25 deg C	İ
Molar Intrinsic Solubility (ISLB.MOL)	0.00000031 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000038 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	:-	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	!-	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	! <b>-</b>	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L		(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	pH 6 25 deg C	
Molar Solubility (SLB.MOL)	0.00000031 mol/L		(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L		(1)
Molar Solubility (SLB.MOL)	0.00000033 mol/L	рн 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000058 mol/L	рн 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	Unbuffered Water	(1)
•		pH 7.00	
	Í	25 deg C	
Molar Volume (MVOL)	408.8+/-3.0 cm**3/mol	20 deg C	(1)
		760 Torr	1
Molecular Weight (MW)	517.57		(1)
pKa (PKA)	10.04+/-0.70	Most Acidic	(1)
		25 deg C	ļ
pKa (PKA)	0.40+/-0.33	Most Basic	(1)
		25 deg C	
Polar Surface Area (PSA)	82.57 A**2		(1)

This substance may exist in multiple tautomeric forms. The property values in this table are calculated based upon the displayed form and may therefore differ from experimental values based on the actual tautomeric ratio at equilibrium.

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

GI

```
ΑN
    125:167581 CA
    Preparation of hydroxybenzamide derivatives as prevention and treatment
ΤI
    agents for bone diseases
    Nomoto, Takashi; Kawakami, Kumiko; Akagawa, Akiko; Matsuyama, Kenji;
IN
    Torigoe, Koichiro
    Banyu Pharma Co Ltd, Japan
PΑ
    Jpn. Kokai Tokkyo Koho, 15 pp.
SO
    CODEN: JKXXAF
DT
    Patent
LA
    Japanese
     ICM C07C235-64
IC
         A61K031-165; A61K031-415; A61K031-44; A61K031-445; A61K031-47;
         A61K031-505; C07C235-56; C07C237-42; C07C255-24; C07D211-06;
         C07D211-22; C07D211-58; C07D213-75; C07D217-06; C07D231-56;
         C07D233-88; C07D239-26; C07D295-18
     25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
CC
     Section cross-reference(s): 1
FAN.CNT 1
                    KIND DATE
     PATENT NO.
                                         APPLICATION NO. DATE
                           -----
     ______
                     _ _ _ -
    JP 08143525
                    A2
                           19960604
                                         JP 1994-311235
                                                          19941121
ΡI
PRAI JP 1994-311235 19941121
```

```
HO CONR<sup>2</sup> (CH<sub>2</sub>) _{n}A
```

DT.CA CAplus document type: Journal

```
The title bone disease inhibitors contain a compound (I) [R1 = H, halo, OH,
AB
     NO2, lower alkyl, lower alkoxy; R2 = H, lower alkyl; n = 0-3; A = aryl,
     heteroaryl; A and R2 may combine to complete piperidine or
     tetrahydroisoquinoline ring]. I is an efficient component for prevention
     and treatment of bone diseases caused by Vacuolar ATPase. Thus,
     2,3,4-tribenzyloxybenzoic acid was reacted with aniline in the presence of
     4-dimethylaminopyridine and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide,
     followed by hydrogenation to give I [R1 = OH; R2 = H; n = 0; A = Ph], 4
     μM of which showed Vacuolar ATPase inhibiting activity of 97%.
     hydroxybenzamide prepn prevention treatment bone disease; Vacuolar ATPase
ST
     inhibitor hydroxybenzamide
     Bone, disease
IT
        (synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)
IT
     9000-83-3
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); BIOL (Biological study)
        (proton-translocating; synthesis of hydroxybenzamide derivs. as
        Vacuolar ATPase inhibitors)
     180206-07-9P
                    180206-26-2P
                                   180206-27-3P
                                                  180206-28-4P
                                                                 180206-29-5P
IT
     180206-30-8P
                    180206-33-1P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation); RACT (Reactant or reagent)
        (synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)
                                   180205-91-8P
                                                  180205-92-9P
                                                                 180205-93-0P
IT
     180205-89-4P
                    180205-90-7P
                                                  180205-97-4P
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     180205-94-1P
                    180205-95-2P
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     180206-20-6P
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                    180206-21-7P
     180206-25-1P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)
                                  88-74-4, o-Nitroaniline
                                                             100-44-7, Benzyl
IT
     62-53-3, Aniline, reactions
                           106-50-3, 1,4-Phenylenediamine, reactions 543-27-1
     chloride, reactions
     , Isobutyl chloroformate
                                573-11-5, 2,3,4-Trimethoxybenzoic acid
     610-02-6, 2,3,4-Trihydroxybenzoic acid
                                             1122-58-3,
     4-Dimethylaminopyridine 10294-33-4, Boron tribromide
                                                              25952-53-8,
     1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride 28675-03-8,
     Dimethylaminoaniline
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)
IT
     180206-31-9P
                    180206-32-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)
     ANSWER 7 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
L5
     69589-68-0 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)
CN
FS
     3D CONCORD
MF
     C18 H14 N4 O2
                  BEILSTEIN*, CA, CAPLUS, CASREACT
     STN Files:
         (*File contains numerically searchable property data)
```

RL.NP Roles from non-patents: PREP (Preparation)

# Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
========	+=======	+========	+========-	+========	+=======
C6	C6	6		46.150.18	2
C4N2	NCNC3	6	C4N2	46.195.39	1

# Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
	+=====================================	+=====================================	+====
Bioconc. Factor (BCF)	29.12	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	38.52	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	39.80	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	39.94	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	39.95	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	39.95	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	39.94	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	39.81	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	38.59	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	29.56	pH 10 25 deg C	(1)
Density (DEN)	1.362+/-0.06 g/cm**3	760 Torr	(1)
Freely Rotatable Bonds (FRB)	3		(1)
H acceptors (HAC)	6	ļ	(1)
H donors (HD)	2	ļ	(1)
Hydrogen Donors/Acceptors Sum	8		(1)
(HDAS)			
Koc (KOC)	355.13	рн 1 25 deg C	(1)
Koc (KOC)	469.73	pH 2 25 deg C	(1)
Koc (KOC)	485.40	pH 3 25 deg C	(1)
Koc (KOC)	487.02	pH 4 25 deg C	(1)
Koc (KOC)	487.18	pH 5 25 deg C	(1)
Koc (KOC)	487.18	pH 6 25 deg C	(1)
Koc (KOC)	487.03	pH 7 25 deg C	(1)
Koc (KOC)	485.49	pH 8 25 deg C	(1)
Koc (KOC)	470.63	pH 9 25 deg C	(1)
Koc (KOC)	360.54	pH 10 25 deg C	(1)
logD (LOGD)	2.27	pH 1 25 deg C	(1)
logD (LOGD)	2.39	pH 2 25 deg C	(1)
logD (LOGD)	2.41	pH 3 25 deg C	(1)
logD (LOGD)	2.41	pH 4 25 deg C	(1)
logD (LOGD)	2.41	pH 5 25 deg C	(1)
logD (LOGD)	2.41	рн 6 25 deg C	(1)
logD (LOGD)	2.41	рн 7 25 deg C	(1)
logD (LOGD)	2.41	рн 8 25 deg C	(1)
logD (LOGD)	2.39	рн 9 25 deg C	(1)
logD (LOGD)	2.28	pH 10 25 deg C	(1)
logP (LOGP)	2.410+/-0.630	25 deg C	(1)

Mass Intrinsic Solubility (ISLB.MASS)	0.020 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	0.028 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.023 g/L	<u> </u>	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	12	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	! -	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	·	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	, =	(1)
Mass Solubility (SLB.MASS)	0.021 g/L	1 E	(1)
Mass Solubility (SLB.MASS)	0.027 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	Unbuffered Water	(1)
	i j	рн 6.96	İ
	İ	25 deg C	İ
Molar Intrinsic Solubility	0.000064 mol/L	25 deg C	(1)
(ISLB.MOL)			
Molar Solubility (SLB.MOL)	0.000088 mol/L	12	(1)
Molar Solubility (SLB.MOL)	0.000066 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000066 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000086 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	Unbuffered Water	(1)
		pH 6.96	}
M-1 77-3 (NEIOT.)	222 6. / 2 0 cm++2/mol	25 deg C  20 deg C	  (1)
Molar Volume (MVOL)	233.6+/-3.0 cm**3/mol	760 Torr	(1)
Malagular Naight (MN)	318.33	700 1011	(1)
Molecular Weight (MW)	10.45+/-0.70	Most Acidic	(1)
pKa (PKA)	10.45+/-0.70	25 deg C	\_/
pKa (PKA)	0.57+/-0.33	Most Basic	(1)
pra (1101)	10.37.7	25 deg C	i `-′
Polar Surface Area (PSA)	83.98 A**2		(1)
10101 0011000 11100 (1011)	1	ľ	

Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 (1) ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

90:121516 CA

Section cross-reference(s): 25

```
Condensation of acetanthranil and phenylanthranil with certain
ΤI
     aminoheterocycles. Attempted preparation of some 2,3-disubstituted
     4(3H)-quinazolinones
AU
     El-Zanfally, S.
     Fac. Pharm., Cairo Univ., Cairo, Egypt
CS
     Egyptian Journal of Pharmaceutical Sciences (1978), Volume Date 1976,
SO
     17(1), 29-34
     CODEN: EJPSBZ; ISSN: 0301-5068
DT
     Journal
LA
     English
```

28-14 (Heterocyclic Compounds (More Than One Hetero Atom))

CC GI

AN

```
R<sup>1</sup> X R I
```

L7

0 S L1

FILE 'CAPLUS' ENTERED AT 14:39:40 ON 14 FEB 2006

```
Treating 2-methyl-4H-3,1-benzoxazin-4-ones (I; X = O; R = Me; R1 = H, Br)
AΒ
     with amines R2NH2 (R2 = 2-pyridyl, 4-antipyrinyl) yielded 35-81% the
     corresponding quinazolinones (I; X = NR2). The reactions were carried out
     by fusing the reactants at 150-60° for 3 h or by refluxing in
     pyridine-dioxane for 2 h. Similar reaction of I (X = O, R = Ph, R1 = H)
     with R2NH2 (R2 = 2-, 3-, or 4-pyridyl; 2-pyrimidinyl, or 4-antipyrinyl)
     gave o-R2NHCOC6H4NHCOPh.
     quinazolinone methyl; benzoxazinone methyl condensation pyridylamine;
ST
     antipyrinylamine condensation benzoxazinone
ΙT
     109-12-6
                462-08-8
                           504-24-5
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation of, with 2-phenyl-3,1-benzoxazin-4-one)
IT
     83-07-8
               504-29-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation of, with 3,1-benzoxazin-4-one)
IT
     19165-25-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation of, with antipyrinylamine)
ΙT
     525-76-8
                1022-46-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation of, with pyridyl- or antipyrinylamine)
IT
     890-03-9P
                 1898-05-1P
                              69589-64-6P
                                             69589-65-7P
                                                           69589-66-8P
     69589-67-9P
                   69589-68-0P
                                69608-79-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
=> d his
     (FILE 'HOME' ENTERED AT 14:36:32 ON 14 FEB 2006)
     FILE 'REGISTRY' ENTERED AT 14:37:27 ON 14 FEB 2006
Ll
                STRUCTURE UPLOADED
L2
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                S L1
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L3
     FILE 'CAPLUS' ENTERED AT 14:38:17 ON 14 FEB 2006
              0 S L3
L4
                S L1
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FILE 'CAPLUS' ENTERED AT 14:40:54 ON 14 FEB 2006

FILE 'REGISTRY' ENTERED AT 14:41:09 ON 14 FEB 2006

FILE 'CAPLUS' ENTERED AT 14:41:13 ON 14 FEB 2006

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:h COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY

SESSION

TOTAL

FULL ESTIMATED COST

0.46 236.75

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

ENTRY 0.00 SESSION -4.97

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:41:32 ON 14 FEB 2006

Connection closed by remote host

G1:0,N

G2:0,[\*1],[\*2]

Match level :

=> s 11 sub sam

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:CLASS

#### L1 STRUCTURE UPLOADED

ENTER SUBSET L# OR (END):ll
L1 MAY NOT BE USED HERE
The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET.
ENTER SUBSET L# OR (END):end
SEARCH ENDED BY USER

=> s l1

SAMPLE SEARCH INITIATED 14:10:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\* PROJECTED ITERATIONS: 106 TO 614 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 0.88 1.09

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FILE COVERS 1907 - 14 Feb 2006 VOL 144 ISS 8 FILE LAST UPDATED: 13 Feb 2006 (20060213/ED)

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=> s 11 sam

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:11:39 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 106 TO 614 PROJECTED ANSWERS: 0 TO 0

0 SEA SSS SAM L1 L3

L4 0 L3

=> s 11

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:12:03 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 0 ANSWERS 18 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 106 TO 614

0 0 TO PROJECTED ANSWERS:

0 SEA SSS SAM L1

0 L5 L6

=> s 11 full REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 14:12:25 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 340 TO ITERATE

100.0% PROCESSED 340 ITERATIONS 7 ANSWERS

SEARCH TIME: 00.00.01

7 SEA SSS FUL L1

1.8

```
ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2000:457059 CAPLUS
DN
     133:89437
     Preparation of heteroaryl-substituted aromatic amides as factor Xa
TI
     inhibitors
     Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman;
IN
     Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven
     Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine
     Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez,
     Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald
     Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton;
     Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PA
     Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SO
     PCT Int. Appl., 403 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
                                                                 DATE
     PATENT NO.
                       KIND
                               DATE
                                         APPLICATION NO.
                        ----
                                          -----
                                                                 -----
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                        A1 20000706 WO 1999-US29946 19991215
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     WO 2000039118
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     CA 2361149
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                                                                 19991215
                               20011010
                                         EP 1999-964279
     EP 1140903
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                                                                 19991215
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                               20040804
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     JP 2002533454
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    US 6635657
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                                                                 20030729
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A1
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    US 2005282862
                               20051222
                                         US 2003-629817
                                                                 20030729
PRAI US 1998-113556P
                               19981223
                         W
     WO 1999-US29946
                               19991215
     US 2001-857751
                         A3
                               20010608
    MARPAT 133:89437
os
             THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 6
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
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    ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
T.A
                        2000:457059 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                        133:89437
ENTRY DATE:
                        Entered STN: 07 Jul 2000
TITLE:
                        Preparation of heteroaryl-substituted aromatic amides
                        as factor Xa inhibitors
                        Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl
INVENTOR(S):
                        Penman; Franciskovich, Jeffry Bernard; Goodson,
                        Theodore, Jr.; Hall, Steven Edward; Herron, David
                        Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine
                        Joseph; Masters, John Joseph; Mendel, David; Milot,
                        Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott;
                        Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe,
                        Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard
                        Crayton; Wikel, James Howard; Wiley, Michael Robert;
```

Yee, Ying Kwong

```
Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
PATENT ASSIGNEE(S):
                        PCT Int. Appl., 403 pp.
SOURCE:
                        CODEN: PIXXD2
DOCUMENT TYPE:
                        Patent
LANGUAGE:
                        English
INT. PATENT CLASSIF.:
                        C07D401-14
           MAIN:
                        C07D401-12; C07D417-14; C07D409-14; C07D405-14;
       SECONDARY:
                        CO7D213-74; A61K031-395; A61K031-435; A61K031-495;
                        A61P007-02; C07D401-14; C07D213-00; C07D213-00;
                        C07D211-00
                        27-16 (Heterocyclic Compounds (One Hetero Atom))
CLASSIFICATION:
                        Section cross-reference(s): 1, 28, 63
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                    KIND DATE
                                      APPLICATION NO. DATE
     PATENT NO.
    WO 2000039118 A1 20000706 WO 1999-US29946 19991215
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            CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
            IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
            MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
            SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
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            CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                        AA 20000706 CA 1999-2361149
                                                                 19991215
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MARPAT 133:89437
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OTHER SOURCE(S): GRAPHIC IMAGE:

#### ABSTRACT:

The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

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SUPPL. TERM: arom amide heteroaryl prepn formulation factor Xa inhibitor anticoagulant
INDEX TERM: Anticoagulants
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(preparation of heteroaryl-substituted aromatic amides as factor

Xa inhibitors)

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(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

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   Xa inhibitors)
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ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
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INDEX TERM:

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(preparation of heteroaryl-substituted aromatic amides as factor
Xa inhibitors)
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INDEX TERM:

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280774-00-7P 280774-01-8P 280774-02-9P 280774-03-0P 280774-04-1P 280774-05-2P 280774-06-3P 280774-07-4P

280774-15-4P 280774-08-5P 280774-09-6P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted aromatic amides as factor

Xa inhibitors)

REFERENCE COUNT: THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD.

(1) Beight Douglas Wade; WO 9900121 A 1999 CAPLUS

(2) Beight Douglas Wade; WO 9900128 A 1999 CAPLUS

(3) Berlex Lab; WO 9628427 A 1996 CAPLUS

(4) Katakura; EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY CHIMICA THERAPEUTICA 1995, V30(5), P387 CAPLUS

(5) Kunitada, S; CURRENT PHARMACEUTICAL DESIGN 1996, V2(5),

(6) Schering Ag; WO 9932477 A 1999 CAPLUS

#### => d ibib abs 1

ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN L8

2000:457059 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 133:89437

TITLE: Preparation of heteroaryl-substituted aromatic amides

as factor Xa inhibitors

Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl INVENTOR(S):

> Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert;

Yee, Ying Kwong

Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al. PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 403 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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WO 1999-US29946 US 2001-857751

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W 19991215 A3 20010608

OTHER SOURCE(S):

MARPAT 133:89437

A5.A6 L1 Q1

The title compds. [I; A3-A6, together with the two carbons to which they AB are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, MeO, etc.; one of R4 and R5 =H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un) substituted at the 6-position, 2-pyrimidinyl (un) substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; <math>Q2 =(un) substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day. REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L1

 $L_3$ 

T.4

L5

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L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000

S L1

S L1

2000:457059 CAPLUS

DOCUMENT NUMBER:

133:89437

TITLE: Preparation of heteroaryl-substituted aromatic amides

as factor Xa inhibitors

INVENTOR(S):

Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong

PATENT ASSIGNEE(S):

Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.

PCT Int. Appl., 403 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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OTHER SOURCE(S):

MARPAT 133:89437

The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

II

CALC

PROP

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The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).
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'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
The following are valid formats:
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fields or predefined formats. The predefined substance formats
are: (RN = CAS Registry Number)
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SAM
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FIDE
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       - FIDE, but only 50 names
IDE
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
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SQD3
       - Same as SQD, but 3-letter amino acid codes are used
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SQN
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Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats

- Table of calculated properties EPROP - Table of experimental properties

- EPROP and CALC

# must be cited first. The CA File predefined formats are: ABS -- Abstract APPS -- Application and Priority Information BIB -- CA Accession Number, plus Bibliographic Data CAN -- CA Accession Number CBIB -- CA Accession Number, plus Bibliographic Data (compressed) IND -- Index Data IPC -- International Patent Classification PATS -- PI, SO STD -- BIB, IPC, and NCL IABS -- ABS, indented, with text labels IBIB -- BIB, indented, with text labels ISTD -- STD format, indented OBIB ----- AN, plus Bibliographic Data (original) OIBIB ----- OBIB, indented with text labels SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available. The MAX format is the same as ALL. The IALL format is the same as ALL with BIB ABS and IND indented, with text labels. For additional information, please consult the following help messages: HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats. ENTER DISPLAY FORMAT (IDE):ide ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN L7 856975-07-0 REGISTRY RNEntered STN: 26 Jul 2005 ED Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) CN INDEX NAME) 3D CONCORD FS MF C20 H18 N4 O4 CAS EARLY REGISTRATIONS SR STN Files: CA, CAPLUS LC $Ph-CH_2-O$ Me \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\* 1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Benzamide, 2-(acetylamino)-N-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA

ANSWER 2 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

349622-99-7 REGISTRY

INDEX NAME)

C15 H16 N4 O2

Chemical Library

3D CONCORD

Entered STN: 01 Aug 2001

L7

RN ED

CN

FS

MF

SR

Supplier: MicroChemistry Ltd.

LC STN Files: CHEMCATS

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 280768-70-9 REGISTRY

ED Entered STN: 27 Jul 2000

CN 4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phe

nyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H21 Cl N6 O2

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 267891-53-2 REGISTRY

ED Entered STN: 02 Jun 2000

CN Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI)

(CA INDEX NAME)

FS 3D CONCORD

MF C21 H16 Cl N5 O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 267891-24-7 REGISTRY

ED Entered STN: 02 Jun 2000

CN Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI)

(CA INDEX NAME)

FS 3D CONCORD

MF C17 H14 C1 N5 O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 180206-29-5 REGISTRY

ED Entered STN: 29 Aug 1996

CN Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX

NAME)

FS 3D CONCORD

MF C32 H27 N3 O4

SR CA

LC STN Files: CA, CAPLUS

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN

RN 69589-68-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H14 N4 O2

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

(\*File contains numerically searchable property data)

=> d 16 hitstr ibib abs 1-7

L6 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

IT 280768-70-9P

RN

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

280768-70-9 CAPLUS

4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phe nyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)

ACCESSION NUMBER: 2000:457059 CAPLUS

DOCUMENT NUMBER: 133:89437

TITLE: Preparation of heteroaryl-substituted aromatic amides

as factor Xa inhibitors

INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl

Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert;

Yee, Ying Kwong

PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.

SOURCE: PCT Int. Appl., 403 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA:	rent :	NO.			KIN	ND DATE													
WO 2000039118					A1	2000070				WO 1	999-1		19991215						
	W:	ΑE,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,		
		CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	ΗU,	ID,	IL,		
		IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,		
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	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZW,	AT,	BE,	CH,	CY,	DE,		
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		CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG						
CA 2361149				AA		2000	0706		CA 1	999-	2361	149		1	9991	215			
EP 1140903														9991	215				
ΕP	1140	903			B1		2004	0804											
							ES,			GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,		
							RO												
JР	2002	5334	54		T2		2002	1008		JP 2	000-		19991215						
AT	2726	33			E		2004	0815			999-					9991	215		
ES	2226	485			Т3		2005	0316		ES 1	999-	9642	79		1	9991	215		
US	US 6635657									US 2	001-	8577	51		20010608				
US	US 2004029874				A1		2004	0212		US 2	003-	6297	60		20030729				
US	6759	414			B2		2004	0706											
US	2005	2828	62		A1		20051222			US 2003-629817						20030729			

PRIORITY APPLN. INFO.:

US 1998-113556P WO 1999-US29946 US 2001-857751

II

19981223 W 19991215 A3 20010608

OTHER SOURCE(S):

MARPAT 133:89437

GI

The title compds. [I; A3-A6, together with the two carbons to which they AB are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 =H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un) substituted at the 5-position, 3-pyridinyl (un) substituted at the 6-position, 2-pyrimidinyl (un) substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un) substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day. THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 6 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN L6

267891-24-7P 267891-53-2P IT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of anthranilic acid amides as VEGF receptor inhibitors)

267891-24-7 CAPLUS RN

Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) CN (CA INDEX NAME)

RN 267891-53-2 CAPLUS

Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) CN (CA INDEX NAME)

ACCESSION NUMBER: 2000:335387 CAPLUS

DOCUMENT NUMBER: 132:334364

TITLE: Preparation of anthranilic acid amides as vascular

endothelial growth factor receptor inhibitors.

INVENTOR(S): Huth, Andreas; Seidelmann, Dieter; Thierauch,

Karl-Heinz; Bold, Guido; Manley, Paul William; Furet,

Pascal; Wood, Jeanette Marjorie; Mestan, Jurgen; Bruggen, Jose; Ferrari, Stefano; Kruger, Martin; Ottow, Eckhard; Menrad, Andreas; Schirner, Michael

Schering Aktiengesellschaft, Germany; Novartis

Aktiengesellschaft

PCT Int. Appl., 96 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

LANGUAGE: Germa: FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT ASSIGNEE(S):

SOURCE:

PAT	ENT	. 01			KIND DATE					APPI	LICAT:		DATE					
WO	2000	A2 20000518			WO 1999-EP8478						19991109							
WO	NO 2000027819				A3 20000817													
										BG,	, BR,	BY,	CA,	CH,	CN,	CR,	CU,	
		CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD	, GE,	GH,	GM,	HR,	HU,	ID,	IL,	
			-								, LK,							
		MD.	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL	, PT,	RO,	RU,	SD,	SE,	SG,	SI,	
											, US,							
							RU,											
	RW:									TZ	, UG,	ZW,	ΑT,	BE,	CH,	CY,	DE,	
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		CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE	, SN,	TD,	TG					
DE 19910396 DE 19910396				A1		2000	0907		DE :	1999-:	1991	0396		19990303				
DE	DE 19910396				C2		2001	1213										
CA 2350208			AΑ		2000	0518		CA :	1999-:	2350	208		1	9991	109			
BR	9915	553			Α	A 20010814				BR :	1999-:		1	9991	109			
EΡ	1129	074			A2	20010905			EP 1999-953967						19991109			
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		ΙE,	SI,	LT,	LV,	FI,	RO											
						T2 20020521							19991109					
JP	2002	5294	52		T2		2002	0910		JP :	2000-	5809	99			9991		
EE	2001	0025	8		Α		2002	1216	EE 2001-258						_	9991		
NZ	5114	13			Α		2004	0130			1999-							
ΑU	7711	80			B2		2004	0318		AU 2000-10454 NO 2001-2245						9991	109	
NO	2001	0022	45		Α		2001	0710										
	1055				Α		2002				2001-					0010	_	
HK	1041	882			A1		2005	0318		HK :	2002-	1036	28		2	0020		
RIT	APP	LN.	INFO	.:						GB :	1998-:	2457	9	•	A 1			
											1999-							
										WO :	1999-1	EP84	78	,	W 1	9991	109	

OTHER SOURCE(S): MARPAT 132:334364

GI

$$R^{5}$$
 $AZR^{1}$ 
 $R^{6}$ 
 $XYR^{3}$ 
 $R^{7}$ 
 $I$ 

AB Title compds. [I; A = NR2; W = O, S, H2, NR8; Z = NR10, N, NR10(CH2)q,
 alkyl, etc.; q = 1-6; AZR1 = tetrahydroisoquinolinyl, indazolyl,
 5-chloroindolyl, etc.; R1 = (substituted) aryl, heteroaryl; R2 = H, alkyl;
 R3 = (substituted) mono- or bicyclic aryl, heteroaryl; R4-R7 = H, halo,
 (substituted) alkoxy, alkyl, carboxyalkyl; R5R6 = dioxetanyl; R8, R10 = H,

 alkyl]. Thus, Me N-(4-pyridylmethyl)anthranilate (preparation given) was stirred with Ph(CH2)3NH2 and Me3Al were stirred in PhMe to give N-(3-phenylprop-1-yl)-N2-(4-pyridylmethyl) anthranilamide. The latter inhibited VEGFR I with IC50 = 0.05  $\mu M$ .

ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN L6 IT

180206-29-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)

RN 180206-29-5 CAPLUS

Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX

ACCESSION NUMBER:

1996:513596 CAPLUS

DOCUMENT NUMBER:

125:167581

TITLE:

Preparation of hydroxybenzamide derivatives as

INVENTOR(S):

CN

prevention and treatment agents for bone diseases Nomoto, Takashi; Kawakami, Kumiko; Akagawa, Akiko;

Matsuyama, Kenji; Torigoe, Koichiro

Banyu Pharma Co Ltd, Japan

PATENT ASSIGNEE(S): SOURCE:

Jpn. Kokai Tokkyo Koho, 15 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

GI

IT

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
JP 08143525	A2	19960604	JP 1994-311235	19941121		
PRIORITY APPLN. INFO.:			JP 1994-311235	19941121		
OTHER SOURCE(S):	MARPAT	125:167581				

CONR2 (CH2) nA

The title bone disease inhibitors contain a compound (I) [R1 = H, halo, OH, AB NO2, lower alkyl, lower alkoxy; R2 = H, lower alkyl; n = 0-3; A = aryl, heteroaryl; A and R2 may combine to complete piperidine or tetrahydroisoquinoline ring]. I is an efficient component for prevention and treatment of bone diseases caused by Vacuolar ATPase. Thus, 2,3,4-tribenzyloxybenzoic acid was reacted with aniline in the presence of 4-dimethylaminopyridine and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide, followed by hydrogenation to give I [R1 = OH; R2 = H; n = 0; A = Ph], 4  $\mu M$  of which showed Vacuolar ATPase inhibiting activity of 97%.

L6 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

I

69589-68-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

ACCESSION NUMBER:

1979:121516 CAPLUS

DOCUMENT NUMBER:

90:121516

TITLE:

Condensation of acetanthranil and phenylanthranil with

certain aminoheterocycles. Attempted preparation of

some 2,3-disubstituted 4(3H)-quinazolinones

AUTHOR (S):

El-Zanfally, S.

CORPORATE SOURCE:

Fac. Pharm., Cairo Univ., Cairo, Egypt

SOURCE:

Egyptian Journal of Pharmaceutical Sciences (1978),

Volume Date 1976, 17(1), 29-34 CODEN: EJPSBZ; ISSN: 0301-5068

DOCUMENT TYPE:

Journal English

LANGUAGE: OTHER SOURCE(S):

CASREACT 90:121516

GI

CN

$$R^1$$
 $X$ 
 $R$ 

Treating 2-methyl-4H-3,1-benzoxazin-4-ones (I; X = O; R = Me; R1 = H, Br) AB with amines R2NH2 (R2 = 2-pyridyl, 4-antipyrinyl) yielded 35-81% the corresponding quinazolinones (I; X = NR2). The reactions were carried out by fusing the reactants at 150-60° for 3 h or by refluxing in pyridine-dioxane for 2 h. Similar reaction of I (X = O, R = Ph, R1 = H) with R2NH2 (R2 = 2-, 3-, or 4-pyridyl; 2-pyrimidinyl, or 4-antipyrinyl) gave o-R2NHCOC6H4NHCOPh.

ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN L6

856975-07-0, Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-IT dimethyl-

(preparation of)

RN 856975-07-0 CAPLUS

Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA CN INDEX NAME)

ACCESSION NUMBER: 1953:22216 CAPLUS

DOCUMENT NUMBER: 47:22216

ORIGINAL REFERENCE NO.: 47:3819d-i,3820a-i

TITLE: Tuberculostatic derivatives of p-aminobenzoic acid.

III. Heterocyclic derivatives of 4-aminosalicylic acid

AUTHOR(S): Jensen, Kai Arne; Ingvorsen, Helmuth

CORPORATE SOURCE: Univ. Copenhagen

SOURCE: Acta Chemica Scandinavica (1952), 6, 161-5

CODEN: ACHSE7; ISSN: 0904-213X

DOCUMENT TYPE: Journal LANGUAGE: English

cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and 4-aminosalicylic acid (II) were prepared, including 4-nitrosalicylomorpholide (III), m. 247-8°, and -piperidide (IV), m. 230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and -piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m. 170° and 4-aminobenzoic acid (VIII), m. 160°; 2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X), m. 178°, and -benzanilide (XI), m. 201°; 4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'nitrobenzamido) pyridine (XIII), m. 144°, -thiazole (XIV), m. 201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4aminobenzamido)pyridine (XVII), m. 183°, -thiazole (XVIII), m. 214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et 4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at 120°, the excess XX removed at 100° in vacuo, the residue dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving 50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g. PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were refluxed until colorless, 0.2 N NaOH added until the color reappeared, the EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction of the NO2 gave VIII. VII (10 g.) and 10 cc. SOCl2 were refluxed 1-1.5 h., the excess SOC12 was removed in vacuo, and the IX (9.2 g.) treated with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in 30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9 g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into 300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the solution filtered, part of the EtOH removed in vacuo, H2O added, the solution heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9 g. acid chloride. XVII to XIX were obtained by hydrogenation of the corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro compds. at 100° and 150 atmospheric gave the corresponding azoxy compds.

AB

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ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
L6
     2000:457059 CAPLUS
AN
     133:89437
DN
     Preparation of heteroaryl-substituted aromatic amides as factor Xa
ΤI
     inhibitors
     Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman;
IN
     Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven
     Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine
     Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez,
     Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald
     Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton;
     Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
     Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
PΑ
     PCT Int. Appl., 403 pp.
SO
     CODEN: PIXXD2
ÐΤ
     Patent
LΑ
     English
FAN.CNT 1
                                         APPLICATION NO.
                                                                 DATE
                     KIND DATE
     WO 2000039118 A1
     PATENT NO.
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                         A1 20000706 WO 1999-US29946 19991215
PΙ
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              IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
         SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
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                                            CA 1999-2361149
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     EP 1140903
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                           В1
                                 20040804
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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                                              JP 2000-591029
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                          T2
     JP 2002533454
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     AT 272633
                                            ES 1999-964279
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                          T3
                                 20050316
     ES 2226485
US 6635657 B1 20031021
US 2004029874 A1 20040212
US 6759414 B2 20040706
US 2005282862 A1 20051222
PRAI US 1998-113556P P 19981223
WO 1999-US29946 W 19991215
US 2001-857751
                                            US 2001-857751
                                                                      20010608
                                             US 2003-629760
                                                                      20030729
                                            US 2003-629817
                                                                      20030729
                                  20010608
     US 2001-857751
                           A3
     MARPAT 133:89437
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RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 16 bib abs hitstr 1-7
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

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ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
L6
     2000:457059 CAPLUS
AN
     133:89437
DN
     Preparation of heteroaryl-substituted aromatic amides as factor Xa
ΤI
     inhibitors
     Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman;
IN
     Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven
     Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine
     Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez,
     Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald
     Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
```

PA Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.

SO PCT Int. Appl., 403 pp.

CODEN: PIXXD2

DT	Patent
LΑ	English
FAN.	CNT 1

RN

CN

2.724.	PATENT	NO.	KIND DATE				APPLICATION NO.							DATE			
ΡI	WO 2000					WO 1999-US29946											
	<b>W</b> :	AE, AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG	3,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
		CZ, DE,	DK,	DM,	EE,	ES,	FI,	GB,	GI	Ο,	GE,	GH,	GM,	HR,	ΗU,	ID,	IL,
		IN, IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC	Ξ,	LK,	LR,	LS,	LT,	LU,	LV,	MA,
		MD, MG,	MK,	MN,	MW,	MX,	NO,	ΝZ,	PΙ	٠, د	PT,	RO,	RU,	SD,	SE,	SG,	SI,
		SK, SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG	3,	US,	UZ,	VN,	ΥU,	ZA,	zw	
	RW:	GH, GM,	KE,	LS,	MW,	SD,	SL,	SZ,	TZ	Ζ,	ŪĠ,	ZW,	AT,	BE,	CH,	CY,	DE,
		DK, ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU	J,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,
		CG, CI,															
	CA 2361		CA 1999-2361149							19991215							
								EP 1999-964279									
		903			0804												
	R:	AT, BE,	CH,	DE,	DK,	ES,	FR,	GB,	GF	₹,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE, SI,	LT,	LV,	FI,	RO											
	JP 2002	533454		T2	JP 2000-591029							19991215					
	AT 2726	33		E		0815	AT 1999-964279							19991215			
	ES 2226	485		Т3	0316	ES 1999-964279							19991215				
	US 6635	657		B1	1021	US 2001-857751							2	0010	608		
		029874				2004	0212	US 2003-629760							2	0030	729
	US 6759	414		B2		2004	0706										
	US 2005	282862		A1		2005	1222		US	20	03-	6298	17		2	0030	729
PRAI	US 1998	-113556F	•	P		1998	1223										
	WO 1999	-US29946		W		1999	1215										
	US 2001	857751		A3		2001	0608										
os	MARPAT	133:8943	7														
GI																	

The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

280768-70-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors) 280768-70-9 CAPLUS

4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phe nyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)

# RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:335387 CAPLUS

DN 132:334364

TI Preparation of anthranilic acid amides as vascular endothelial growth factor receptor inhibitors.

IN Huth, Andreas; Seidelmann, Dieter; Thierauch, Karl-Heinz; Bold, Guido; Manley, Paul William; Furet, Pascal; Wood, Jeanette Marjorie; Mestan, Jurgen; Bruggen, Jose; Ferrari, Stefano; Kruger, Martin; Ottow, Eckhard; Menrad, Andreas; Schirner, Michael

PA Schering Aktiengesellschaft, Germany; Novartis Aktiengesellschaft

SO PCT Int. Appl., 96 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 2

os

GI

MARPAT 132:334364

FAN.			NO.									APPLICATION NO.								
							-													
PI					A2		2000	0518	WO 1999-EP8478							19991109				
	WO	20000	0278	19		<b>A</b> 3		2000												
		W:	ΑE,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG	3, B	BR,	BY,	CA,	CH,	CN,	CR,	CU,	
								ES,												
								ΚP,												
								MX,												
			SK,	SL,	ТJ,	TM,	TR,	ΤT,	TZ,	UA,	UG, U		ß,	UZ,	VN,	YU,	ZA,	ZW,	AM,	
								RU,												
		RW:						SD,												
								GR,								SE,	BF,	ВJ,	CF,	
			CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	NE	E, S	SN,	TD,	TG					
	DE 19910396 A1					A1		2000	0907	DE 1999-19910396							19990303			
	DΕ	1991	0396			C2		2001	1213											
	CA	CA 2350208						2000	0518		CA 1999-2350208 BR 1999-15553						19991109			
	ВR	9915	553			A		2001	0814		BR	199	9-	1555	3		19	9991:	109	
	ΕP						20010905													
		R:	ΑT,	ΒE,	CH,	DE,	DK,	ES,	FR,	GB,	GF	₹, I	Τ,	LI,	LU,	ΝL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FI,	RO								_				
	TR	2001	0130	7		T2		2002	TR 2001-200101307 JP 2000-580999							19991109				
	JP	2002	5294	52		T2		2002	0910	JP 2000-580999							13	<del>9</del> 991.	109	
	$\mathbf{E}\mathbf{E}$	2001	0025	8		A		2002	1216	EE 2001-258							Т;	9991.	109	
		5114	13			A B2		2004										9991		
		77118	В0			B2		2004									1:	999I.	109	
	МО	2001	0022	45		Α		2001	0710		NO 2001-2245 BG 2001-105588									
	ВG	1055	88			Α														
	HK	1041	882			Al		2005			нк	200	)2-	1036	28		2	3020	514	
PRAI		1998						1998												
	DE	1999	-199	1039	6	A														
	WO	1999	-EP8	478		W		1999	1109											

Title compds. [I; A = NR2; W = O, S, H2, NR8; Z = NR10, N, NR10(CH2)q, alkyl, etc.; q = 1-6; AZR1 = tetrahydroisoquinolinyl, indazolyl, 5-chloroindolyl, etc.; R1 = (substituted) aryl, heteroaryl; R2 = H, alkyl; R3 = (substituted) mono- or bicyclic aryl, heteroaryl; R4-R7 = H, halo, (substituted) alkoxy, alkyl, carboxyalkyl; R5R6 = dioxetanyl; R8, R10 = H, alkyl]. Thus, Me N-(4-pyridylmethyl)anthranilate (preparation given) was stirred with Ph(CH2)3NH2 and Me3Al were stirred in PhMe to give N-(3-phenylprop-1-yl)-N2-(4-pyridylmethyl)anthranilamide. The latter inhibited VEGFR I with IC50 = 0.05  $\mu$ M.

IT 267891-24-7P 267891-53-2P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of anthranilic acid amides as VEGF receptor inhibitors)

267891-24-7 CAPLUS

RN

RN

I

CN Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)

267891-53-2 CAPLUS

CN Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)

- L6 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1996:513596 CAPLUS
- DN 125:167581
- TI Preparation of hydroxybenzamide derivatives as prevention and treatment agents for bone diseases
- IN Nomoto, Takashi; Kawakami, Kumiko; Akagawa, Akiko; Matsuyama, Kenji; Torigoe, Koichiro

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Banyu Pharma Co Ltd, Japan
PA
    Jpn. Kokai Tokkyo Koho, 15 pp.
SO
    CODEN: JKXXAF
DT
    Patent
    Japanese
FAN.CNT 1
                       KIND
    PATENT NO.
                             DATE
                                        APPLICATION NO.
                                                             DATE
                                        ------
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                                        JP 1994-311235
                       A2
                             19960604
                                                             19941121
    JP 08143525
PΙ
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19941121

PRAI JP 1994-311235

MARPAT 125:167581

os

GI

AB The title bone disease inhibitors contain a compound (I) [R1 = H, halo, OH, NO2, lower alkyl, lower alkoxy; R2 = H, lower alkyl; n = 0-3; A = aryl, heteroaryl; A and R2 may combine to complete piperidine or tetrahydroisoquinoline ring]. I is an efficient component for prevention and treatment of bone diseases caused by Vacuolar ATPase. Thus, 2,3,4-tribenzyloxybenzoic acid was reacted with aniline in the presence of 4-dimethylaminopyridine and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide, followed by hydrogenation to give I [R1 = OH; R2 = H; n = 0; A = Ph], 4 μM of which showed Vacuolar ATPase inhibiting activity of 97%.

180206-29-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors) 180206-29-5 CAPLUS

RN 180206-29-5 CAPLUS
CN Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

L6 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

Ι

AN 1979:121516 CAPLUS

DN 90:121516

TI Condensation of acetanthranil and phenylanthranil with certain aminoheterocycles. Attempted preparation of some 2,3-disubstituted 4(3H)-quinazolinones

El-Zanfally, S.

CS Fac. Pharm., Cairo Univ., Cairo, Egypt

SO Egyptian Journal of Pharmaceutical Sciences (1978), Volume Date 1976, 17(1), 29-34

CODEN: EJPSBZ; ISSN: 0301-5068

DT Journal

LA English

OS CASREACT 90:121516

GI

ΑU

Treating 2-methyl-4H-3,1-benzoxazin-4-ones (I; X = O; R = Me; R1 = H, Br) AΒ with amines R2NH2 (R2 = 2-pyridyl, 4-antipyrinyl) yielded 35-81% the corresponding quinazolinones (I; X = NR2). The reactions were carried out by fusing the reactants at 150-60° for 3 h or by refluxing in pyridine-dioxane for 2 h. Similar reaction of I (X = O, R = Ph, R1 = H) with R2NH2 (R2 = 2-, 3-, or 4-pyridyl; 2-pyrimidinyl, or 4-antipyrinyl) gave o-R2NHCOC6H4NHCOPh.

69589-68-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

RN 69589-68-0 CAPLUS

Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME) CN

1953:22216 CAPLUS

47:22216 OREF 47:3819d-i,3820a-i

L6 ΑN

DN

```
Tuberculostatic derivatives of p-aminobenzoic acid. III. Heterocyclic
TI
     derivatives of 4-aminosalicylic acid
ΑU
     Jensen, Kai Arne; Ingvorsen, Helmuth
CS
    Univ. Copenhagen
SO
    Acta Chemica Scandinavica (1952), 6, 161-5
    CODEN: ACHSE7; ISSN: 0904-213X
DT
    Journal
LΑ
    English
    cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and
AB
     4-aminosalicylic acid (II) were prepared, including 4-nitro-
     salicylomorpholide (III), m. 247-8°, and -piperidide (IV), m.
     230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and
     -piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m.
     170° and 4-aminobenzoic acid (VIII), m. 160°;
     2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X),
     m. 178°, and -benzanilide (XI), m. 201°;
     4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'-
    nitrobenzamido) pyridine (XIII), m. 144°, -thiazole (XIV), m.
     201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and
     -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4-
     aminobenzamido) pyridine (XVII), m. 183°, -thiazole (XVIII), m.
     214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et
     4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at
     120°, the excess XX removed at 100° in vacuo, the residue
     dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving
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50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g. PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were refluxed until colorless, 0.2 N NaOH added until the color reappeared, the EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction of the NO2 gave VIII. VII (10 g.) and 10 cc. SOCl2 were refluxed 1-1.5 h., the excess SOCl2 was removed in vacuo, and the IX (9.2 g.) treated with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in 30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9 g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into 300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the solution filtered, part of the EtOH removed in vacuo, H2O added, the solution heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9 g. acid chloride. XVII to XIX were obtained by hydrogenation of the corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro compds. at 100° and 150 atmospheric gave the corresponding azoxy compds. 856975-07-0, Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6dimethyl-

(preparation of)

IT

RN

CN

856975-07-0 CAPLUS

Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA INDEX NAME)